Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 06:31 PM EDT

PDB ID	:	2MSR
BMRB ID	:	25130
Title	:	Solution structure of LEDGF/p75 IBD in complex with MLL1 peptide (140-160)
Authors	:	Cermakova, K.; Tesina, P.; Demeulemeester, J.; El Ashkar, S.; Mereau, H.; Schwaller, J.; Rezacova, P.; Veverka, V.; De Rijck, J.
Deposited on	:	2014-08-05

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

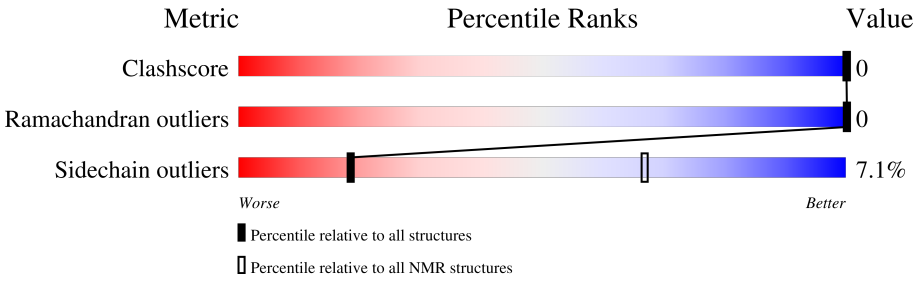
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	21	100%
2	B	88	85% · 13%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	B:348-B:424 (77)	0.53	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 8 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 11, 14
2	7, 9, 10, 15
3	6, 16
Single-model clusters	4; 8; 12; 13; 17; 18; 19; 20

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1750 atoms, of which 880 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone-lysine N-methyltransferase 2A.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	21	296	95	137	28	36	0

- Molecule 2 is a protein called PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	88	1454	438	743	131	135	7	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	SER	-	expression tag	UNP O75475
B	340	ASN	-	expression tag	UNP O75475
B	341	ALA	-	expression tag	UNP O75475
B	342	ALA	-	expression tag	UNP O75475
B	343	SER	-	expression tag	UNP O75475

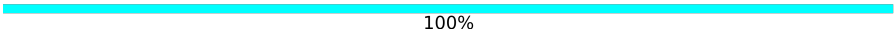
4 Residue-property plots

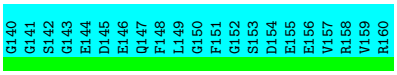
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Histone-lysine N-methyltransferase 2A

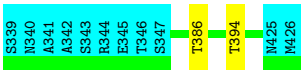
Chain A:





• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:



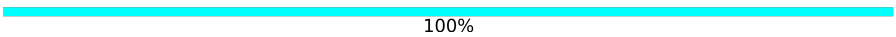
4.2 Scores per residue for each member of the ensemble

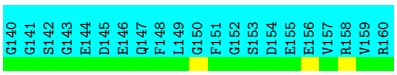
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:





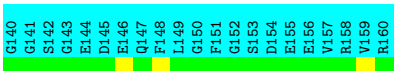
• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:

4.2.2 Score per residue for model 2 (medoid)

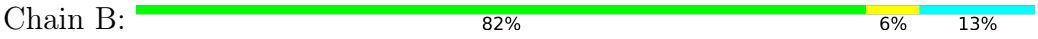
• Molecule 1: Histone-lysine N-methyltransferase 2A

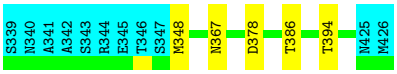
Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:

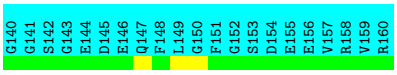




4.2.3 Score per residue for model 3

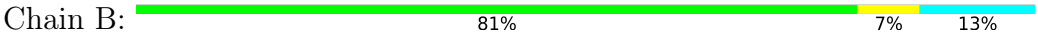
• Molecule 1: Histone-lysine N-methyltransferase 2A

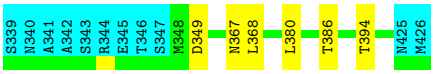
Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:





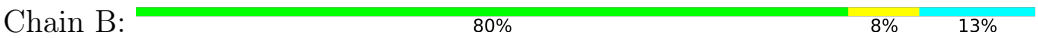
4.2.4 Score per residue for model 4

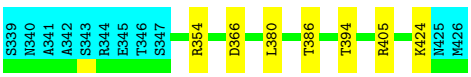
• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:

• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:

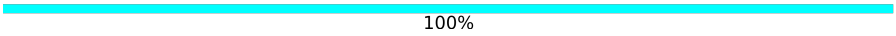


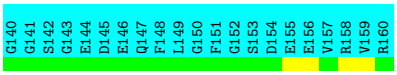


4.2.5 Score per residue for model 5

• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:





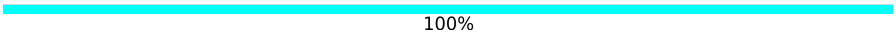
• Molecule 2: PC4 and SFRS1-interacting protein

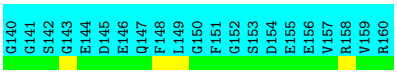
Chain B:

4.2.6 Score per residue for model 6

• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:





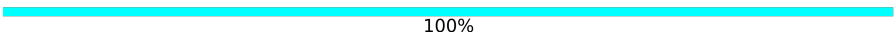
• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:

4.2.7 Score per residue for model 7

• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:



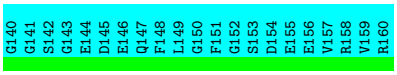
• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:

4.2.8 Score per residue for model 8

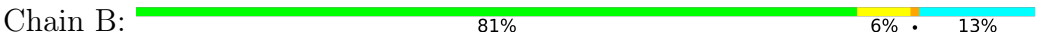
• Molecule 1: Histone-lysine N-methyltransferase 2A

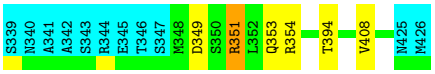
Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:

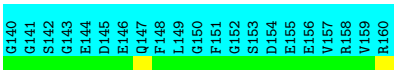




4.2.9 Score per residue for model 9

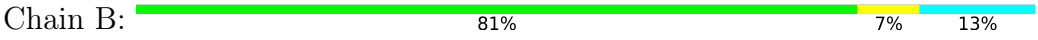
• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

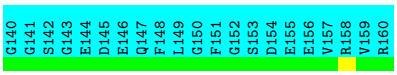
Chain B:



4.2.10 Score per residue for model 10

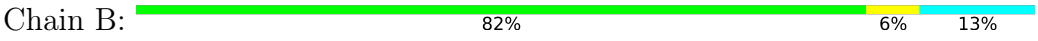
• Molecule 1: Histone-lysine N-methyltransferase 2A

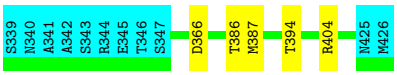
Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:

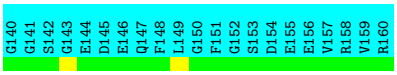




4.2.11 Score per residue for model 11

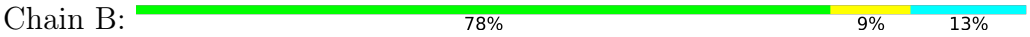
• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

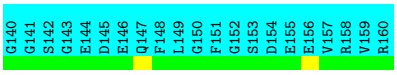
Chain B:



4.2.12 Score per residue for model 12

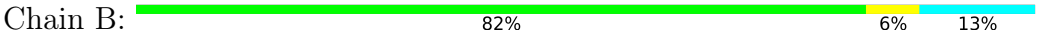
• Molecule 1: Histone-lysine N-methyltransferase 2A

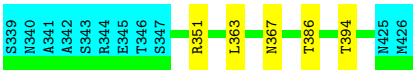
Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:





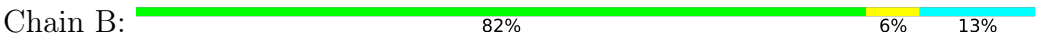
4.2.13 Score per residue for model 13

• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:

• Molecule 2: PC4 and SFRS1-interacting protein

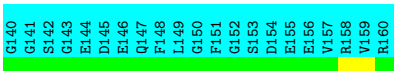
Chain B:



4.2.14 Score per residue for model 14

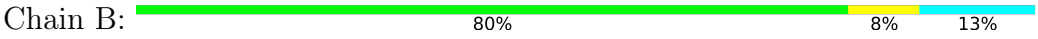
• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

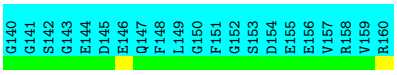
Chain B:



4.2.15 Score per residue for model 15

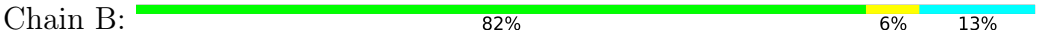
• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:



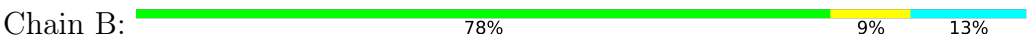
4.2.16 Score per residue for model 16

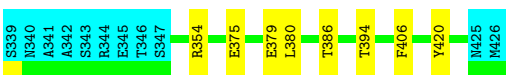
• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:

• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:

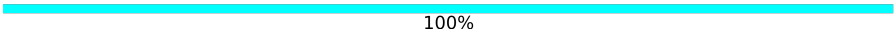


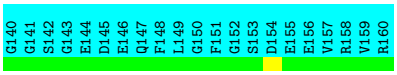


4.2.17 Score per residue for model 17

• Molecule 1: Histone-lysine N-methyltransferase 2A

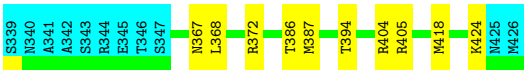
Chain A:





• Molecule 2: PC4 and SFRS1-interacting protein

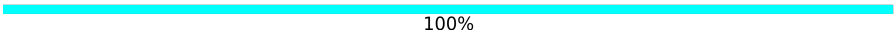
Chain B:

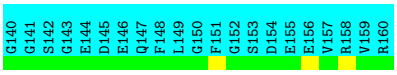


4.2.18 Score per residue for model 18

• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:





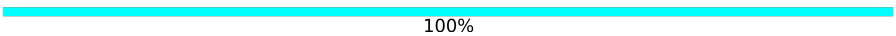
• Molecule 2: PC4 and SFRS1-interacting protein

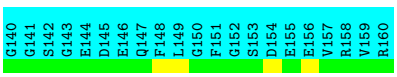
Chain B:

4.2.19 Score per residue for model 19

• Molecule 1: Histone-lysine N-methyltransferase 2A

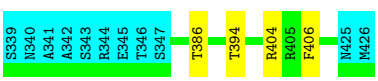
Chain A:





• Molecule 2: PC4 and SFRS1-interacting protein

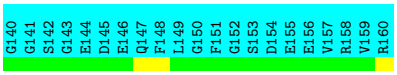
Chain B:



4.2.20 Score per residue for model 20

• Molecule 1: Histone-lysine N-methyltransferase 2A

Chain A:



• Molecule 2: PC4 and SFRS1-interacting protein

Chain B:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, molecular dynamics.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	
YASARA	refinement	
CYANA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1195
Number of shifts mapped to atoms	1195
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
2	B	0.66±0.16	0±0/637 (0.0± 0.1%)	0.69±0.07	1±1/850 (0.1± 0.1%)
All	All	0.67	3/12740 (0.0%)	0.70	17/17000 (0.1%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	375	GLU	CD-OE1	-5.20	1.20	1.25	16	1
2	B	420	TYR	CG-CD2	5.16	1.45	1.39	20	1
2	B	420	TYR	CD2-CE2	5.06	1.47	1.39	16	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	404	ARG	NE-CZ-NH1	6.13	123.37	120.30	13	5
2	B	372	ARG	NE-CZ-NH1	6.08	123.34	120.30	20	5
2	B	354	ARG	NE-CZ-NH1	5.88	123.24	120.30	14	5
2	B	351	ARG	NE-CZ-NH1	5.66	123.13	120.30	20	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	12640	13440	13440	-

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is -.

There are no clashes.

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	0	-	-	-	-
2	B	77/88 (88%)	74±1 (96±1%)	3±1 (4±1%)	0±0 (0±0%)	100 100
All	All	1540/2180 (71%)	1485 (96%)	55 (4%)	0 (0%)	100 100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	0	-	-	-
2	B	73/82 (89%)	68±1 (93±2%)	5±1 (7±2%)	18 67
All	All	1460/1960 (74%)	1356 (93%)	104 (7%)	18 67

All 28 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	394	THR	19
2	B	386	THR	14

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Mol	Chain	Res	Type	Models (Total)
2	B	367	ASN	8
2	B	380	LEU	7
2	B	372	ARG	5
2	B	378	ASP	5
2	B	368	LEU	4
2	B	366	ASP	4
2	B	349	ASP	3
2	B	405	ARG	3
2	B	424	LYS	3
2	B	418	MET	3
2	B	354	ARG	3
2	B	406	PHE	3
2	B	379	GLU	2
2	B	363	LEU	2
2	B	389	GLN	2
2	B	351	ARG	2
2	B	387	MET	2
2	B	369	ASP	2
2	B	362	SER	1
2	B	348	MET	1
2	B	377	LEU	1
2	B	353	GLN	1
2	B	408	VAL	1
2	B	388	GLN	1
2	B	410	GLN	1
2	B	404	ARG	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1195
Number of shifts mapped to atoms	1195
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	87	-0.53 ± 0.11	Should be checked
$^{13}C_{\beta}$	87	0.36 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	82	-0.11 ± 0.12	None needed (< 0.5 ppm)
^{15}N	83	-0.19 ± 0.30	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 998 atoms were assigned a chemical shift out of a possible 1138. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	380/385 (99%)	152/154 (99%)	152/154 (99%)	76/77 (99%)
Sidechain	603/710 (85%)	411/459 (90%)	187/217 (86%)	5/34 (15%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	15/43 (35%)	14/22 (64%)	1/19 (5%)	0/2 (0%)
Overall	998/1138 (88%)	577/635 (91%)	340/390 (87%)	81/113 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1191 atoms were assigned a chemical shift out of a possible 1522. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	456/550 (83%)	204/223 (91%)	169/218 (78%)	83/109 (76%)
Sidechain	710/909 (78%)	502/584 (86%)	202/279 (72%)	6/46 (13%)
Aromatic	25/63 (40%)	24/32 (75%)	1/29 (3%)	0/2 (0%)
Overall	1191/1522 (78%)	730/839 (87%)	372/526 (71%)	89/157 (57%)

7.1.4 Statistically unusual chemical shifts (i)

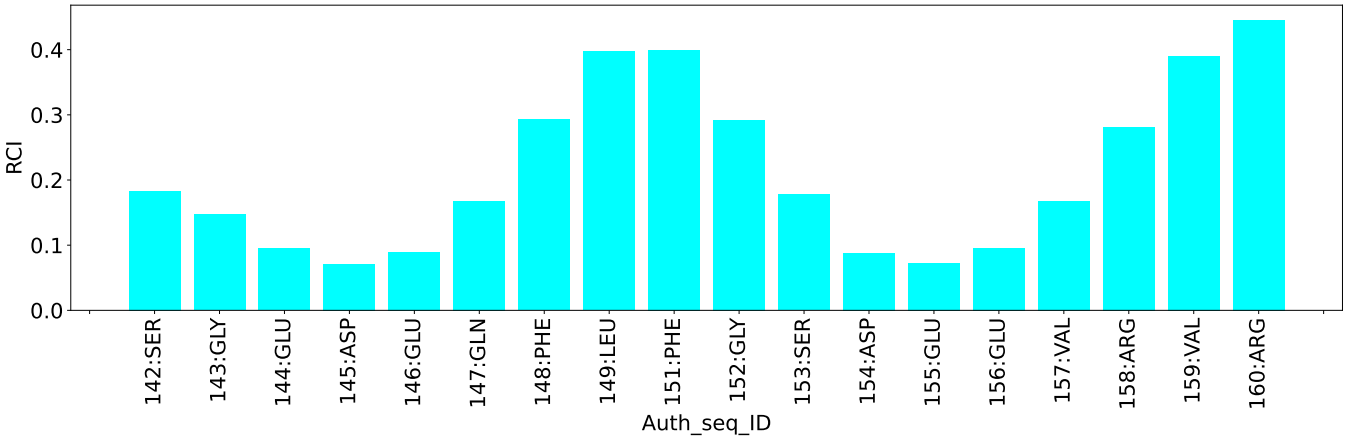
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	417	THR	HG1	5.57	0.08 – 2.19	21.0
1	B	386	THR	HG1	5.53	0.08 – 2.19	20.8

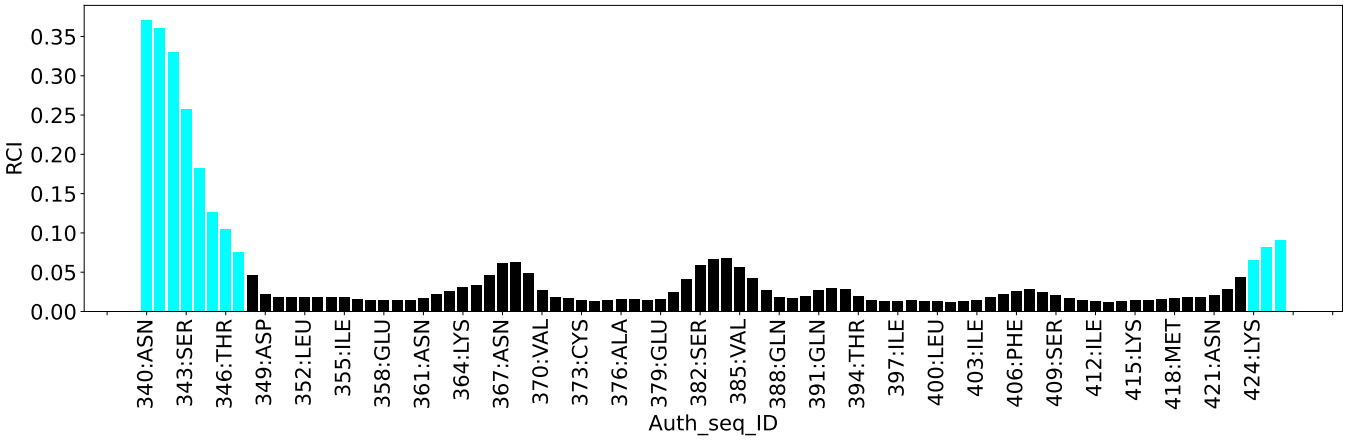
7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1319
Intra-residue (|i-j|=0)	450
Sequential (|i-j|=1)	301
Medium range (|i-j|>1 and |i-j|<5)	279
Long range (|i-j|≥5)	250
Inter-chain	39
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	138
Number of unmapped restraints	0
Number of restraints per residue	13.4
Number of long range restraints per residue[1]	2.3

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	3.8	0.2
0.2-0.5 (Medium)	2.3	0.5
>0.5 (Large)	2.0	1.83

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.9	5.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

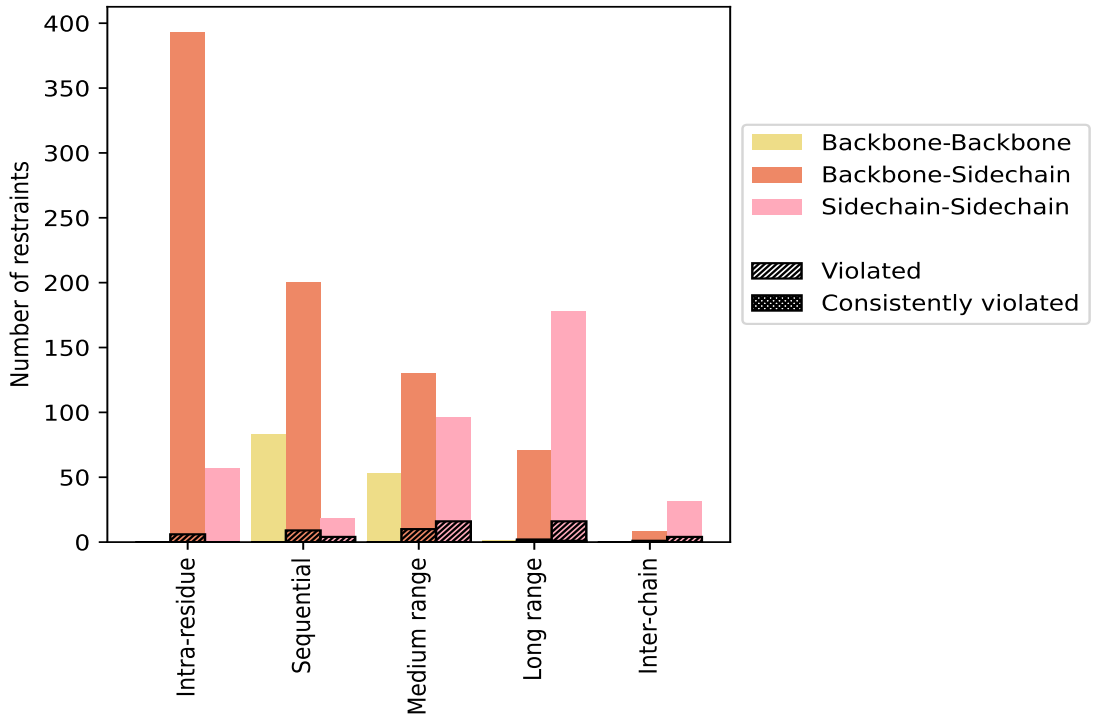
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	450	34.1	6	1.3	0.5	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	393	29.8	6	1.5	0.5	0	0.0	0.0
Sidechain-Sidechain	57	4.3	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	301	22.8	13	4.3	1.0	0	0.0	0.0
Backbone-Backbone	83	6.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	200	15.2	9	4.5	0.7	0	0.0	0.0
Sidechain-Sidechain	18	1.4	4	22.2	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	279	21.2	26	9.3	2.0	0	0.0	0.0
Backbone-Backbone	53	4.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	130	9.9	10	7.7	0.8	0	0.0	0.0
Sidechain-Sidechain	96	7.3	16	16.7	1.2	0	0.0	0.0
Long range (|i-j|≥5)	250	19.0	18	7.2	1.4	2	0.8	0.2
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	71	5.4	2	2.8	0.2	1	1.4	0.1
Sidechain-Sidechain	178	13.5	16	9.0	1.2	1	0.6	0.1
Inter-chain	39	3.0	5	12.8	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	0.6	1	12.5	0.1	0	0.0	0.0
Sidechain-Sidechain	31	2.4	4	12.9	0.3	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1319	100.0	68	5.2	5.2	2	0.2	0.2
Backbone-Backbone	137	10.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	802	60.8	28	3.5	2.1	1	0.1	0.1
Sidechain-Sidechain	380	28.8	40	10.5	3.0	1	0.3	0.1

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	1	1	3	0	5	0.57	1.36	0.46	0.42
2	0	2	2	3	0	7	0.42	1.32	0.39	0.34
3	0	1	1	3	0	5	0.58	1.3	0.52	0.21
4	0	1	0	4	0	5	0.68	1.51	0.58	0.44
5	0	2	1	4	0	7	0.37	1.29	0.4	0.14
6	0	1	0	4	0	5	0.64	1.43	0.43	0.49
7	0	3	1	2	1	7	0.5	1.55	0.48	0.25
8	0	1	1	4	0	6	0.33	0.52	0.15	0.3
9	0	2	4	3	1	10	0.42	1.47	0.39	0.22
10	1	1	1	2	0	5	0.6	1.37	0.41	0.49
11	0	3	1	3	0	7	0.41	1.4	0.42	0.22

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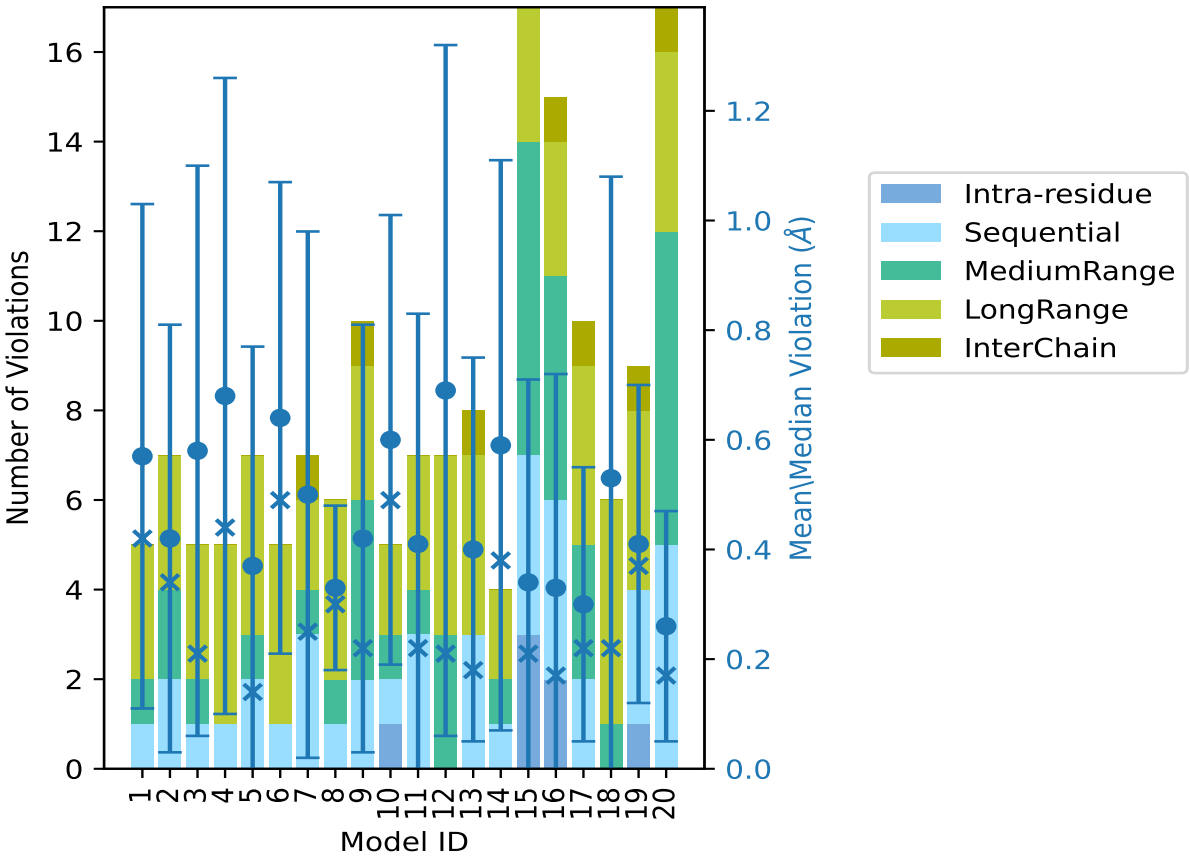
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	3	4	0	7	0.69	1.83	0.63	0.21
13	0	3	0	4	1	8	0.4	0.97	0.35	0.18
14	0	1	1	2	0	4	0.59	1.47	0.52	0.38
15	3	4	7	3	0	17	0.34	1.73	0.37	0.21
16	2	4	5	3	1	15	0.33	1.44	0.39	0.17
17	0	2	3	4	1	10	0.3	0.94	0.25	0.22
18	0	0	1	5	0	6	0.53	1.61	0.55	0.22
19	1	3	0	4	1	9	0.41	1.01	0.29	0.37
20	0	5	7	4	1	17	0.26	0.98	0.21	0.17

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

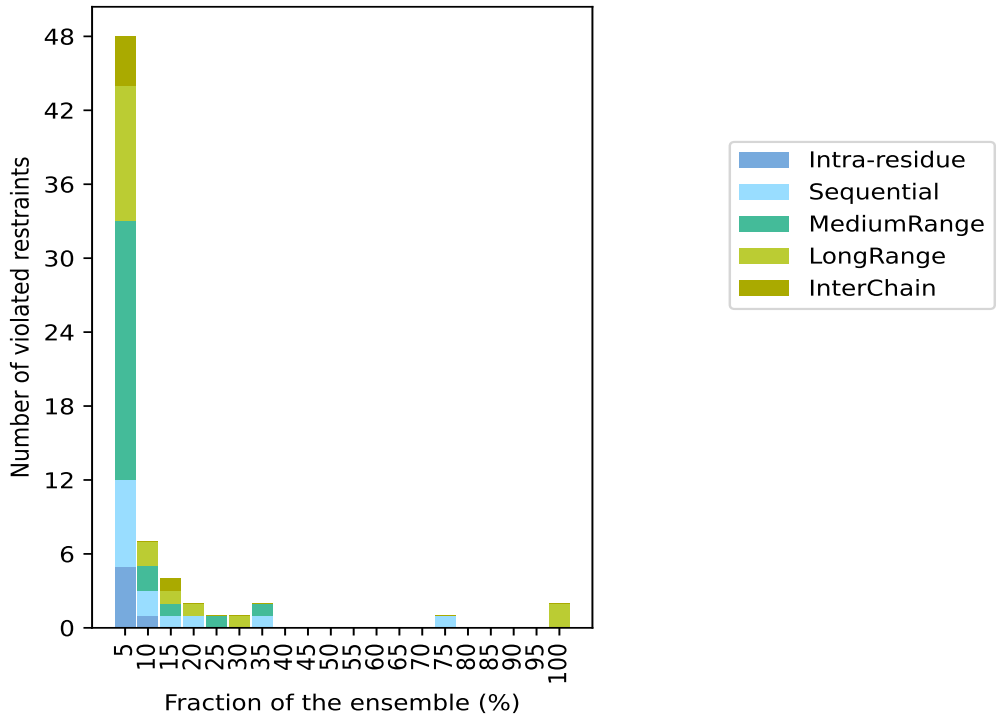
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1251(IR:444, SQ:288, MR:253, LR:232, IC:34) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
5	7	21	11	4	48	1	5.0
1	2	2	2	0	7	2	10.0
0	1	1	1	1	4	3	15.0
0	1	0	1	0	2	4	20.0
0	0	1	0	0	1	5	25.0
0	0	0	1	0	1	6	30.0
0	1	1	0	0	2	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	1	0	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	2	0	2	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

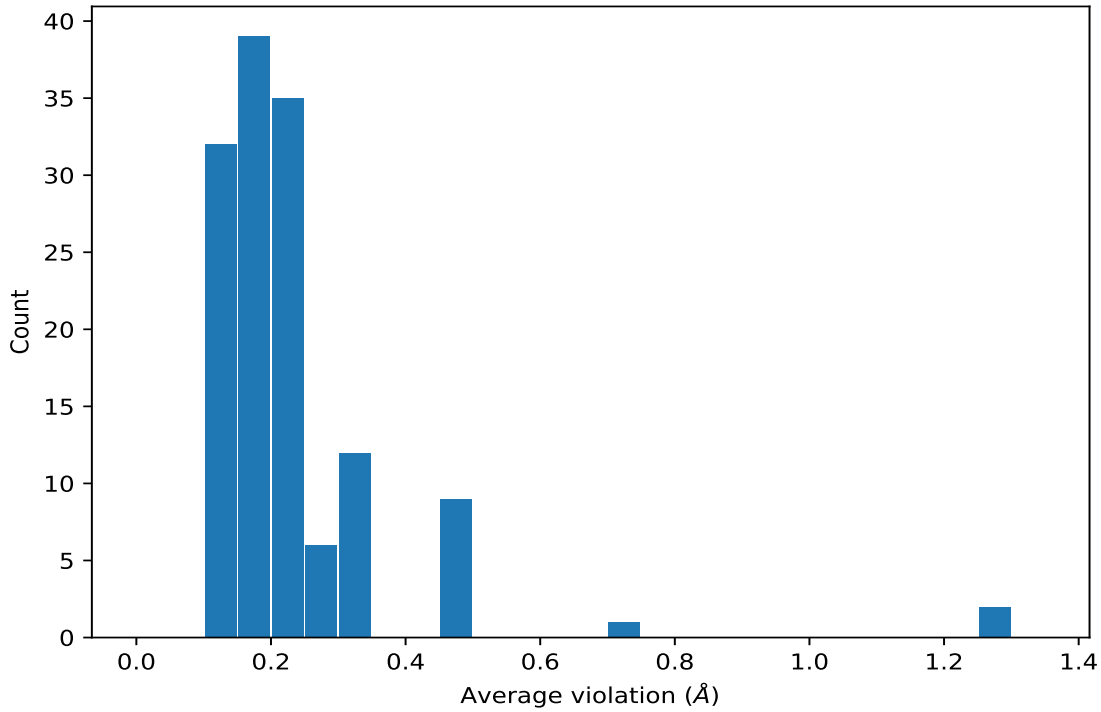
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	20	1.29	0.29	1.37
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	20	1.29	0.29	1.37
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	20	0.72	0.38	0.62
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	15	0.49	0.06	0.49
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	15	0.49	0.06	0.49
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	15	0.49	0.06	0.49
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	15	0.49	0.06	0.49
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	15	0.49	0.06	0.49
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	15	0.49	0.06	0.49
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD11	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD12	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD13	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD11	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD12	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD13	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD11	7	0.23	0.13	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD12	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD13	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD11	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD12	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD13	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD11	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD12	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD13	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD11	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD12	7	0.23	0.13	0.18
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD13	7	0.23	0.13	0.18
(1,173)	2:B:368:LEU:HD11	2:B:369:ASP:H	7	0.14	0.03	0.13
(1,173)	2:B:368:LEU:HD12	2:B:369:ASP:H	7	0.14	0.03	0.13
(1,173)	2:B:368:LEU:HD13	2:B:369:ASP:H	7	0.14	0.03	0.13
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE1	6	0.46	0.28	0.35
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE2	6	0.46	0.28	0.35
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE3	6	0.46	0.28	0.35
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD11	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD12	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD13	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD21	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD22	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD23	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD11	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD12	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD13	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD21	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD22	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD23	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD11	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD12	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD13	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD21	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD22	5	0.14	0.03	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD23	5	0.14	0.03	0.12
(1,311)	2:B:405:ARG:H	2:B:406:PHE:HB2	4	0.17	0.06	0.16
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE1	4	0.14	0.02	0.13
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE2	4	0.14	0.02	0.13
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE3	4	0.14	0.02	0.13
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE1	4	0.14	0.02	0.13
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE2	4	0.14	0.02	0.13
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE3	4	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE1	4	0.14	0.02	0.13
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE2	4	0.14	0.02	0.13
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE3	4	0.14	0.02	0.13
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG11	3	0.28	0.07	0.25
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG12	3	0.28	0.07	0.25
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG13	3	0.28	0.07	0.25
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG11	3	0.28	0.07	0.25
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG12	3	0.28	0.07	0.25
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG13	3	0.28	0.07	0.25
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG11	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG12	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG13	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG21	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG22	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG23	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG11	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG12	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG13	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG21	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG22	3	0.22	0.13	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG23	3	0.22	0.13	0.13
(1,1269)	2:B:411:VAL:HG11	2:B:415:LYS:HD2	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG11	2:B:415:LYS:HD3	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG12	2:B:415:LYS:HD2	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG12	2:B:415:LYS:HD3	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG13	2:B:415:LYS:HD2	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG13	2:B:415:LYS:HD3	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG21	2:B:415:LYS:HD2	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG21	2:B:415:LYS:HD3	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG22	2:B:415:LYS:HD2	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG22	2:B:415:LYS:HD3	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG23	2:B:415:LYS:HD2	3	0.19	0.03	0.17
(1,1269)	2:B:411:VAL:HG23	2:B:415:LYS:HD3	3	0.19	0.03	0.17
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE1	3	0.16	0.06	0.13
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE2	3	0.16	0.06	0.13
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE3	3	0.16	0.06	0.13
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE1	3	0.16	0.06	0.13
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE2	3	0.16	0.06	0.13
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE3	3	0.16	0.06	0.13
(1,1055)	2:B:368:LEU:HD11	2:B:406:PHE:HE1	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD11	2:B:406:PHE:HE2	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD12	2:B:406:PHE:HE1	2	0.31	0.18	0.31

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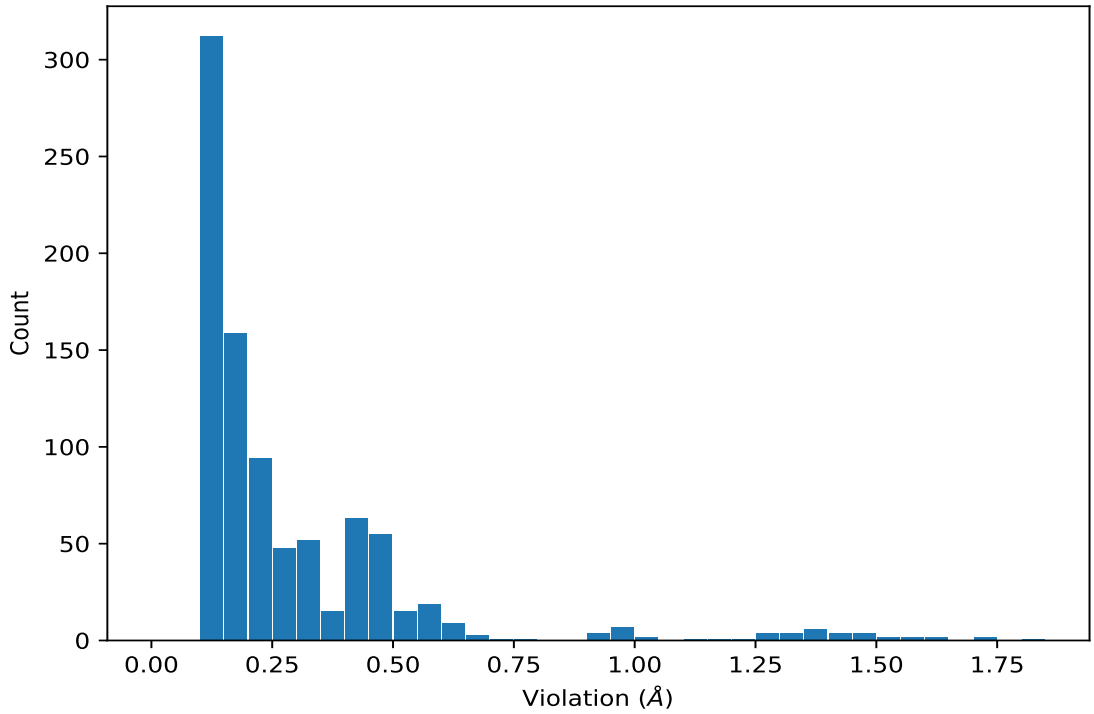
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1055)	2:B:368:LEU:HD12	2:B:406:PHE:HE2	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD13	2:B:406:PHE:HE1	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD13	2:B:406:PHE:HE2	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD21	2:B:406:PHE:HE1	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD21	2:B:406:PHE:HE2	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD22	2:B:406:PHE:HE1	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD22	2:B:406:PHE:HE2	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD23	2:B:406:PHE:HE1	2	0.31	0.18	0.31
(1,1055)	2:B:368:LEU:HD23	2:B:406:PHE:HE2	2	0.31	0.18	0.31
(1,1019)	2:B:362:SER:HA	2:B:364:LYS:HG2	2	0.24	0.07	0.24
(1,1019)	2:B:362:SER:HA	2:B:364:LYS:HG3	2	0.24	0.07	0.24
(1,452)	2:B:393:HIS:H	2:B:396:MET:HE1	2	0.2	0.08	0.2
(1,452)	2:B:393:HIS:H	2:B:396:MET:HE2	2	0.2	0.08	0.2
(1,452)	2:B:393:HIS:H	2:B:396:MET:HE3	2	0.2	0.08	0.2
(1,386)	2:B:420:TYR:HE1	2:B:421:ASN:H	2	0.19	0.08	0.19
(1,386)	2:B:420:TYR:HE2	2:B:421:ASN:H	2	0.19	0.08	0.19
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD11	2	0.17	0.03	0.17
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD12	2	0.17	0.03	0.17
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD13	2	0.17	0.03	0.17
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD21	2	0.17	0.03	0.17
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD22	2	0.17	0.03	0.17
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD23	2	0.17	0.03	0.17
(1,1121)	2:B:377:LEU:HD11	2:B:415:LYS:HE2	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD11	2:B:415:LYS:HE3	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD12	2:B:415:LYS:HE2	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD12	2:B:415:LYS:HE3	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD13	2:B:415:LYS:HE2	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD13	2:B:415:LYS:HE3	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD21	2:B:415:LYS:HE2	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD21	2:B:415:LYS:HE3	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD22	2:B:415:LYS:HE2	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD22	2:B:415:LYS:HE3	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD23	2:B:415:LYS:HE2	2	0.16	0.04	0.16
(1,1121)	2:B:377:LEU:HD23	2:B:415:LYS:HE3	2	0.16	0.04	0.16
(1,39)	1:A:148:PHE:H	1:A:149:LEU:HB2	2	0.14	0.02	0.14
(1,39)	1:A:148:PHE:H	1:A:149:LEU:HB3	2	0.14	0.02	0.14

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	12	1.83
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	15	1.73
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	15	1.73
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	18	1.61
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	18	1.61
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	7	1.55
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	7	1.55
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	4	1.51
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	4	1.51
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	9	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	9	1.47
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	14	1.47
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	14	1.47
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	16	1.44
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	16	1.44
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	6	1.43
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	6	1.43
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	11	1.4
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	11	1.4
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	10	1.37
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	10	1.37
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	1	1.36
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	1	1.36
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	2	1.32
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	2	1.32
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	3	1.3
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	3	1.3
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	5	1.29
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	5	1.29
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	12	1.29
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	12	1.29
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	4	1.22
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	16	1.19
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	3	1.12
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	19	1.01
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	19	1.01
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	20	0.98
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	20	0.98
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE1	12	0.98
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE2	12	0.98
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE3	12	0.98
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	13	0.97
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	13	0.97
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	17	0.94
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	17	0.94
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	13	0.9
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	18	0.9
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	1	0.76
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	7	0.71
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE1	19	0.65
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE2	19	0.65
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE3	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	6	0.64
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	9	0.64
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	19	0.61
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	13	0.61
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	13	0.61
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	13	0.61
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	13	0.61
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	13	0.61
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	13	0.61
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	9	0.6
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	9	0.6
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	9	0.6
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	9	0.6
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	9	0.6
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	9	0.6
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	11	0.57
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	15	0.56
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	15	0.56
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	15	0.56
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	15	0.56
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	15	0.56
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	15	0.56
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	7	0.55
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	7	0.55
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	7	0.55
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	7	0.55
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	7	0.55
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	7	0.55
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	10	0.54
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	17	0.54
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	17	0.54
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	17	0.54
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	17	0.54
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	17	0.54
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	17	0.54
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	8	0.52
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	8	0.51
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	8	0.51
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	8	0.51
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	8	0.51
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	8	0.51
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	20	0.5
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	6	0.49
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	6	0.49
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	6	0.49
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	6	0.49
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	6	0.49
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	6	0.49
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	10	0.49
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	10	0.49
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	10	0.49
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	10	0.49
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	10	0.49
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	10	0.49
(1,1055)	2:B:368:LEU:HD11	2:B:406:PHE:HE1	6	0.49
(1,1055)	2:B:368:LEU:HD11	2:B:406:PHE:HE2	6	0.49
(1,1055)	2:B:368:LEU:HD12	2:B:406:PHE:HE1	6	0.49
(1,1055)	2:B:368:LEU:HD12	2:B:406:PHE:HE2	6	0.49
(1,1055)	2:B:368:LEU:HD13	2:B:406:PHE:HE1	6	0.49
(1,1055)	2:B:368:LEU:HD13	2:B:406:PHE:HE2	6	0.49
(1,1055)	2:B:368:LEU:HD21	2:B:406:PHE:HE1	6	0.49
(1,1055)	2:B:368:LEU:HD21	2:B:406:PHE:HE2	6	0.49
(1,1055)	2:B:368:LEU:HD22	2:B:406:PHE:HE1	6	0.49
(1,1055)	2:B:368:LEU:HD22	2:B:406:PHE:HE2	6	0.49
(1,1055)	2:B:368:LEU:HD23	2:B:406:PHE:HE1	6	0.49
(1,1055)	2:B:368:LEU:HD23	2:B:406:PHE:HE2	6	0.49
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD11	10	0.47
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD12	10	0.47
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD13	10	0.47
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD11	10	0.47
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD12	10	0.47
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD13	10	0.47
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD11	10	0.47
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD12	10	0.47
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD13	10	0.47
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD11	10	0.47
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD12	10	0.47
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD13	10	0.47
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD11	10	0.47
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD12	10	0.47
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD13	10	0.47
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD11	10	0.47
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD12	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD13	10	0.47
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	2	0.46
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	2	0.46
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	2	0.46
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	2	0.46
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	2	0.46
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	2	0.46
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	2	0.46
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	19	0.46
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	19	0.46
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	19	0.46
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	19	0.46
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	19	0.46
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	19	0.46
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	15	0.44
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	4	0.44
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	4	0.44
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	4	0.44
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	4	0.44
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	4	0.44
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	4	0.44
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	5	0.44
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	5	0.44
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	5	0.44
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	5	0.44
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	5	0.44
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	5	0.44
(1,51)	1:A:147:GLN:HG2	1:A:149:LEU:HD21	15	0.43
(1,51)	1:A:147:GLN:HG2	1:A:149:LEU:HD22	15	0.43
(1,51)	1:A:147:GLN:HG2	1:A:149:LEU:HD23	15	0.43
(1,51)	1:A:147:GLN:HG3	1:A:149:LEU:HD21	15	0.43
(1,51)	1:A:147:GLN:HG3	1:A:149:LEU:HD22	15	0.43
(1,51)	1:A:147:GLN:HG3	1:A:149:LEU:HD23	15	0.43
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	14	0.43
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	14	0.43
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	14	0.43
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	14	0.43
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	14	0.43
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	14	0.43
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	1	0.42
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	1	0.42
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	1	0.42
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	1	0.42
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	1	0.42
(1,964)	2:B:351:ARG:HG2	2:B:383:LEU:HB3	8	0.41
(1,964)	2:B:351:ARG:HG3	2:B:383:LEU:HB3	8	0.41
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD11	9	0.41
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD12	9	0.41
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD13	9	0.41
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD11	9	0.41
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD12	9	0.41
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD13	9	0.41
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD11	9	0.41
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD12	9	0.41
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD13	9	0.41
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD11	9	0.41
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD12	9	0.41
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD13	9	0.41
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD11	9	0.41
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD12	9	0.41
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD13	9	0.41
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD11	9	0.41
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD12	9	0.41
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD13	9	0.41
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG11	15	0.4
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG12	15	0.4
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG13	15	0.4
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG21	15	0.4
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG22	15	0.4
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG23	15	0.4
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG11	15	0.4
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG12	15	0.4
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG13	15	0.4
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG21	15	0.4
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG22	15	0.4
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG23	15	0.4
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG21	20	0.39
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG22	20	0.39
(1,1232)	2:B:402:LYS:HG2	2:B:403:ILE:HG23	20	0.39
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG21	20	0.39
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG22	20	0.39
(1,1232)	2:B:402:LYS:HG3	2:B:403:ILE:HG23	20	0.39
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG11	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG12	19	0.37
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG13	19	0.37
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG11	19	0.37
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG12	19	0.37
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG13	19	0.37
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE1	5	0.36
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE2	5	0.36
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE3	5	0.36
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE1	2	0.34
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE2	2	0.34
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE3	2	0.34
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	14	0.33
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	17	0.32
(1,503)	2:B:386:THR:HG21	2:B:390:ALA:HB1	20	0.32
(1,503)	2:B:386:THR:HG21	2:B:390:ALA:HB2	20	0.32
(1,503)	2:B:386:THR:HG21	2:B:390:ALA:HB3	20	0.32
(1,503)	2:B:386:THR:HG22	2:B:390:ALA:HB1	20	0.32
(1,503)	2:B:386:THR:HG22	2:B:390:ALA:HB2	20	0.32
(1,503)	2:B:386:THR:HG22	2:B:390:ALA:HB3	20	0.32
(1,503)	2:B:386:THR:HG23	2:B:390:ALA:HB1	20	0.32
(1,503)	2:B:386:THR:HG23	2:B:390:ALA:HB2	20	0.32
(1,503)	2:B:386:THR:HG23	2:B:390:ALA:HB3	20	0.32
(1,1028)	2:B:363:LEU:HD11	2:B:368:LEU:HD11	16	0.32
(1,1028)	2:B:363:LEU:HD11	2:B:368:LEU:HD12	16	0.32
(1,1028)	2:B:363:LEU:HD11	2:B:368:LEU:HD13	16	0.32
(1,1028)	2:B:363:LEU:HD11	2:B:368:LEU:HD21	16	0.32
(1,1028)	2:B:363:LEU:HD11	2:B:368:LEU:HD22	16	0.32
(1,1028)	2:B:363:LEU:HD11	2:B:368:LEU:HD23	16	0.32
(1,1028)	2:B:363:LEU:HD12	2:B:368:LEU:HD11	16	0.32
(1,1028)	2:B:363:LEU:HD12	2:B:368:LEU:HD12	16	0.32
(1,1028)	2:B:363:LEU:HD12	2:B:368:LEU:HD13	16	0.32
(1,1028)	2:B:363:LEU:HD12	2:B:368:LEU:HD21	16	0.32
(1,1028)	2:B:363:LEU:HD12	2:B:368:LEU:HD22	16	0.32
(1,1028)	2:B:363:LEU:HD12	2:B:368:LEU:HD23	16	0.32
(1,1028)	2:B:363:LEU:HD13	2:B:368:LEU:HD11	16	0.32
(1,1028)	2:B:363:LEU:HD13	2:B:368:LEU:HD12	16	0.32
(1,1028)	2:B:363:LEU:HD13	2:B:368:LEU:HD13	16	0.32
(1,1028)	2:B:363:LEU:HD13	2:B:368:LEU:HD21	16	0.32
(1,1028)	2:B:363:LEU:HD13	2:B:368:LEU:HD22	16	0.32
(1,1028)	2:B:363:LEU:HD13	2:B:368:LEU:HD23	16	0.32
(1,1028)	2:B:363:LEU:HD21	2:B:368:LEU:HD11	16	0.32
(1,1028)	2:B:363:LEU:HD21	2:B:368:LEU:HD12	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1028)	2:B:363:LEU:HD21	2:B:368:LEU:HD13	16	0.32
(1,1028)	2:B:363:LEU:HD21	2:B:368:LEU:HD21	16	0.32
(1,1028)	2:B:363:LEU:HD21	2:B:368:LEU:HD22	16	0.32
(1,1028)	2:B:363:LEU:HD21	2:B:368:LEU:HD23	16	0.32
(1,1028)	2:B:363:LEU:HD22	2:B:368:LEU:HD11	16	0.32
(1,1028)	2:B:363:LEU:HD22	2:B:368:LEU:HD12	16	0.32
(1,1028)	2:B:363:LEU:HD22	2:B:368:LEU:HD13	16	0.32
(1,1028)	2:B:363:LEU:HD22	2:B:368:LEU:HD21	16	0.32
(1,1028)	2:B:363:LEU:HD22	2:B:368:LEU:HD22	16	0.32
(1,1028)	2:B:363:LEU:HD22	2:B:368:LEU:HD23	16	0.32
(1,1028)	2:B:363:LEU:HD23	2:B:368:LEU:HD11	16	0.32
(1,1028)	2:B:363:LEU:HD23	2:B:368:LEU:HD12	16	0.32
(1,1028)	2:B:363:LEU:HD23	2:B:368:LEU:HD13	16	0.32
(1,1028)	2:B:363:LEU:HD23	2:B:368:LEU:HD21	16	0.32
(1,1028)	2:B:363:LEU:HD23	2:B:368:LEU:HD22	16	0.32
(1,1028)	2:B:363:LEU:HD23	2:B:368:LEU:HD23	16	0.32
(1,1019)	2:B:362:SER:HA	2:B:364:LYS:HG2	15	0.31
(1,1019)	2:B:362:SER:HA	2:B:364:LYS:HG3	15	0.31
(1,1256)	2:B:410:GLN:HB2	2:B:411:VAL:HG11	20	0.28
(1,1256)	2:B:410:GLN:HB2	2:B:411:VAL:HG12	20	0.28
(1,1256)	2:B:410:GLN:HB2	2:B:411:VAL:HG13	20	0.28
(1,1256)	2:B:410:GLN:HB2	2:B:411:VAL:HG21	20	0.28
(1,1256)	2:B:410:GLN:HB2	2:B:411:VAL:HG22	20	0.28
(1,1256)	2:B:410:GLN:HB2	2:B:411:VAL:HG23	20	0.28
(1,1256)	2:B:410:GLN:HB3	2:B:411:VAL:HG11	20	0.28
(1,1256)	2:B:410:GLN:HB3	2:B:411:VAL:HG12	20	0.28
(1,1256)	2:B:410:GLN:HB3	2:B:411:VAL:HG13	20	0.28
(1,1256)	2:B:410:GLN:HB3	2:B:411:VAL:HG21	20	0.28
(1,1256)	2:B:410:GLN:HB3	2:B:411:VAL:HG22	20	0.28
(1,1256)	2:B:410:GLN:HB3	2:B:411:VAL:HG23	20	0.28
(1,452)	2:B:393:HIS:H	2:B:396:MET:HE1	15	0.27
(1,452)	2:B:393:HIS:H	2:B:396:MET:HE2	15	0.27
(1,452)	2:B:393:HIS:H	2:B:396:MET:HE3	15	0.27
(1,386)	2:B:420:TYR:HE1	2:B:421:ASN:H	16	0.27
(1,386)	2:B:420:TYR:HE2	2:B:421:ASN:H	16	0.27
(1,311)	2:B:405:ARG:H	2:B:406:PHE:HB2	20	0.26
(1,965)	2:B:351:ARG:HG2	2:B:383:LEU:HD11	18	0.25
(1,965)	2:B:351:ARG:HG2	2:B:383:LEU:HD12	18	0.25
(1,965)	2:B:351:ARG:HG2	2:B:383:LEU:HD13	18	0.25
(1,965)	2:B:351:ARG:HG2	2:B:383:LEU:HD21	18	0.25
(1,965)	2:B:351:ARG:HG2	2:B:383:LEU:HD22	18	0.25
(1,965)	2:B:351:ARG:HG2	2:B:383:LEU:HD23	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	2:B:351:ARG:HG3	2:B:383:LEU:HD11	18	0.25
(1,965)	2:B:351:ARG:HG3	2:B:383:LEU:HD12	18	0.25
(1,965)	2:B:351:ARG:HG3	2:B:383:LEU:HD13	18	0.25
(1,965)	2:B:351:ARG:HG3	2:B:383:LEU:HD21	18	0.25
(1,965)	2:B:351:ARG:HG3	2:B:383:LEU:HD22	18	0.25
(1,965)	2:B:351:ARG:HG3	2:B:383:LEU:HD23	18	0.25
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE1	17	0.25
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE2	17	0.25
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE3	17	0.25
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE1	17	0.25
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE2	17	0.25
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE3	17	0.25
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG11	7	0.25
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG12	7	0.25
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG13	7	0.25
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG11	7	0.25
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG12	7	0.25
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG13	7	0.25
(1,423)	2:B:348:MET:HE1	2:B:351:ARG:HD2	17	0.25
(1,423)	2:B:348:MET:HE1	2:B:351:ARG:HD3	17	0.25
(1,423)	2:B:348:MET:HE2	2:B:351:ARG:HD2	17	0.25
(1,423)	2:B:348:MET:HE2	2:B:351:ARG:HD3	17	0.25
(1,423)	2:B:348:MET:HE3	2:B:351:ARG:HD2	17	0.25
(1,423)	2:B:348:MET:HE3	2:B:351:ARG:HD3	17	0.25
(1,1269)	2:B:411:VAL:HG11	2:B:415:LYS:HD2	9	0.24
(1,1269)	2:B:411:VAL:HG11	2:B:415:LYS:HD3	9	0.24
(1,1269)	2:B:411:VAL:HG12	2:B:415:LYS:HD2	9	0.24
(1,1269)	2:B:411:VAL:HG12	2:B:415:LYS:HD3	9	0.24
(1,1269)	2:B:411:VAL:HG13	2:B:415:LYS:HD2	9	0.24
(1,1269)	2:B:411:VAL:HG13	2:B:415:LYS:HD3	9	0.24
(1,1269)	2:B:411:VAL:HG21	2:B:415:LYS:HD2	9	0.24
(1,1269)	2:B:411:VAL:HG21	2:B:415:LYS:HD3	9	0.24
(1,1269)	2:B:411:VAL:HG22	2:B:415:LYS:HD2	9	0.24
(1,1269)	2:B:411:VAL:HG22	2:B:415:LYS:HD3	9	0.24
(1,1269)	2:B:411:VAL:HG23	2:B:415:LYS:HD2	9	0.24
(1,1269)	2:B:411:VAL:HG23	2:B:415:LYS:HD3	9	0.24
(1,1185)	2:B:388:GLN:HA	2:B:391:GLN:HG2	16	0.24
(1,1185)	2:B:388:GLN:HA	2:B:391:GLN:HG3	16	0.24
(1,513)	2:B:386:THR:HG21	2:B:388:GLN:HB2	20	0.23
(1,513)	2:B:386:THR:HG22	2:B:388:GLN:HB2	20	0.23
(1,513)	2:B:386:THR:HG23	2:B:388:GLN:HB2	20	0.23
(1,601)	2:B:355:ILE:HD11	2:B:380:LEU:HB2	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	2:B:355:ILE:HD12	2:B:380:LEU:HB2	11	0.22
(1,601)	2:B:355:ILE:HD13	2:B:380:LEU:HB2	11	0.22
(1,1242)	2:B:407:LYS:HG2	2:B:408:VAL:HG11	11	0.22
(1,1242)	2:B:407:LYS:HG2	2:B:408:VAL:HG12	11	0.22
(1,1242)	2:B:407:LYS:HG2	2:B:408:VAL:HG13	11	0.22
(1,1242)	2:B:407:LYS:HG2	2:B:408:VAL:HG21	11	0.22
(1,1242)	2:B:407:LYS:HG2	2:B:408:VAL:HG22	11	0.22
(1,1242)	2:B:407:LYS:HG2	2:B:408:VAL:HG23	11	0.22
(1,1242)	2:B:407:LYS:HG3	2:B:408:VAL:HG11	11	0.22
(1,1242)	2:B:407:LYS:HG3	2:B:408:VAL:HG12	11	0.22
(1,1242)	2:B:407:LYS:HG3	2:B:408:VAL:HG13	11	0.22
(1,1242)	2:B:407:LYS:HG3	2:B:408:VAL:HG21	11	0.22
(1,1242)	2:B:407:LYS:HG3	2:B:408:VAL:HG22	11	0.22
(1,1242)	2:B:407:LYS:HG3	2:B:408:VAL:HG23	11	0.22
(1,946)	1:A:151:PHE:HE1	2:B:402:LYS:HG2	13	0.21
(1,946)	1:A:151:PHE:HE1	2:B:402:LYS:HG3	13	0.21
(1,946)	1:A:151:PHE:HE2	2:B:402:LYS:HG2	13	0.21
(1,946)	1:A:151:PHE:HE2	2:B:402:LYS:HG3	13	0.21
(1,935)	1:A:147:GLN:HE21	1:A:149:LEU:HD11	12	0.21
(1,935)	1:A:147:GLN:HE21	1:A:149:LEU:HD12	12	0.21
(1,935)	1:A:147:GLN:HE21	1:A:149:LEU:HD13	12	0.21
(1,935)	1:A:147:GLN:HE21	1:A:149:LEU:HD21	12	0.21
(1,935)	1:A:147:GLN:HE21	1:A:149:LEU:HD22	12	0.21
(1,935)	1:A:147:GLN:HE21	1:A:149:LEU:HD23	12	0.21
(1,935)	1:A:147:GLN:HE22	1:A:149:LEU:HD11	12	0.21
(1,935)	1:A:147:GLN:HE22	1:A:149:LEU:HD12	12	0.21
(1,935)	1:A:147:GLN:HE22	1:A:149:LEU:HD13	12	0.21
(1,935)	1:A:147:GLN:HE22	1:A:149:LEU:HD21	12	0.21
(1,935)	1:A:147:GLN:HE22	1:A:149:LEU:HD22	12	0.21
(1,935)	1:A:147:GLN:HE22	1:A:149:LEU:HD23	12	0.21
(1,703)	2:B:364:LYS:H	2:B:364:LYS:HD2	15	0.21
(1,703)	2:B:364:LYS:H	2:B:364:LYS:HD3	15	0.21
(1,616)	2:B:374:ILE:HA	2:B:377:LEU:HD21	20	0.21
(1,616)	2:B:374:ILE:HA	2:B:377:LEU:HD22	20	0.21
(1,616)	2:B:374:ILE:HA	2:B:377:LEU:HD23	20	0.21
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG11	16	0.21
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG12	16	0.21
(1,500)	1:A:148:PHE:HD1	2:B:408:VAL:HG13	16	0.21
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG11	16	0.21
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG12	16	0.21
(1,500)	1:A:148:PHE:HD2	2:B:408:VAL:HG13	16	0.21
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE1	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE2	3	0.21
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE3	3	0.21
(1,167)	2:B:364:LYS:HE2	2:B:365:ILE:H	15	0.21
(1,167)	2:B:364:LYS:HE3	2:B:365:ILE:H	15	0.21
(1,54)	1:A:151:PHE:HA	1:A:151:PHE:HE1	15	0.2
(1,54)	1:A:151:PHE:HA	1:A:151:PHE:HE2	15	0.2
(1,50)	1:A:147:GLN:HB2	1:A:149:LEU:HD21	9	0.2
(1,50)	1:A:147:GLN:HB2	1:A:149:LEU:HD22	9	0.2
(1,50)	1:A:147:GLN:HB2	1:A:149:LEU:HD23	9	0.2
(1,50)	1:A:147:GLN:HB3	1:A:149:LEU:HD21	9	0.2
(1,50)	1:A:147:GLN:HB3	1:A:149:LEU:HD22	9	0.2
(1,50)	1:A:147:GLN:HB3	1:A:149:LEU:HD23	9	0.2
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE1	8	0.2
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE2	8	0.2
(1,441)	2:B:352:LEU:HB3	2:B:396:MET:HE3	8	0.2
(1,311)	2:B:405:ARG:H	2:B:406:PHE:HB2	11	0.2
(1,1121)	2:B:377:LEU:HD11	2:B:415:LYS:HE2	9	0.2
(1,1121)	2:B:377:LEU:HD11	2:B:415:LYS:HE3	9	0.2
(1,1121)	2:B:377:LEU:HD12	2:B:415:LYS:HE2	9	0.2
(1,1121)	2:B:377:LEU:HD12	2:B:415:LYS:HE3	9	0.2
(1,1121)	2:B:377:LEU:HD13	2:B:415:LYS:HE2	9	0.2
(1,1121)	2:B:377:LEU:HD13	2:B:415:LYS:HE3	9	0.2
(1,1121)	2:B:377:LEU:HD21	2:B:415:LYS:HE2	9	0.2
(1,1121)	2:B:377:LEU:HD21	2:B:415:LYS:HE3	9	0.2
(1,1121)	2:B:377:LEU:HD22	2:B:415:LYS:HE2	9	0.2
(1,1121)	2:B:377:LEU:HD22	2:B:415:LYS:HE3	9	0.2
(1,1121)	2:B:377:LEU:HD23	2:B:415:LYS:HE2	9	0.2
(1,1121)	2:B:377:LEU:HD23	2:B:415:LYS:HE3	9	0.2
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD11	16	0.2
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD12	16	0.2
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD13	16	0.2
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD21	16	0.2
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD22	16	0.2
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD23	16	0.2
(1,426)	2:B:418:MET:HA	2:B:418:MET:HE1	19	0.19
(1,426)	2:B:418:MET:HA	2:B:418:MET:HE2	19	0.19
(1,426)	2:B:418:MET:HA	2:B:418:MET:HE3	19	0.19
(1,1226)	2:B:401:LYS:HB2	2:B:420:TYR:HD1	12	0.19
(1,1226)	2:B:401:LYS:HB2	2:B:420:TYR:HD2	12	0.19
(1,1226)	2:B:401:LYS:HB3	2:B:420:TYR:HD1	12	0.19
(1,1226)	2:B:401:LYS:HB3	2:B:420:TYR:HD2	12	0.19
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD11	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD12	15	0.19
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD13	15	0.19
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD21	15	0.19
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD22	15	0.19
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD23	15	0.19
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD11	15	0.19
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD12	15	0.19
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD13	15	0.19
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD21	15	0.19
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD22	15	0.19
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD23	15	0.19
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD11	15	0.19
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD12	15	0.19
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD13	15	0.19
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD21	15	0.19
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD22	15	0.19
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD23	15	0.19
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD11	18	0.19
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD12	18	0.19
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD13	18	0.19
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD11	18	0.19
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD12	18	0.19
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD13	18	0.19
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD11	18	0.19
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD12	18	0.19
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD13	18	0.19
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD11	18	0.19
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD12	18	0.19
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD13	18	0.19
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD11	18	0.19
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD12	18	0.19
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD13	18	0.19
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD11	18	0.19
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD12	18	0.19
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD13	18	0.19
(1,498)	2:B:406:PHE:HD1	2:B:408:VAL:HG11	8	0.18
(1,498)	2:B:406:PHE:HD1	2:B:408:VAL:HG12	8	0.18
(1,498)	2:B:406:PHE:HD1	2:B:408:VAL:HG13	8	0.18
(1,498)	2:B:406:PHE:HD2	2:B:408:VAL:HG11	8	0.18
(1,498)	2:B:406:PHE:HD2	2:B:408:VAL:HG12	8	0.18
(1,498)	2:B:406:PHE:HD2	2:B:408:VAL:HG13	8	0.18
(1,484)	2:B:363:LEU:HD21	2:B:412:ILE:HD11	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	2:B:363:LEU:HD21	2:B:412:ILE:HD12	15	0.18
(1,484)	2:B:363:LEU:HD21	2:B:412:ILE:HD13	15	0.18
(1,484)	2:B:363:LEU:HD22	2:B:412:ILE:HD11	15	0.18
(1,484)	2:B:363:LEU:HD22	2:B:412:ILE:HD12	15	0.18
(1,484)	2:B:363:LEU:HD22	2:B:412:ILE:HD13	15	0.18
(1,484)	2:B:363:LEU:HD23	2:B:412:ILE:HD11	15	0.18
(1,484)	2:B:363:LEU:HD23	2:B:412:ILE:HD12	15	0.18
(1,484)	2:B:363:LEU:HD23	2:B:412:ILE:HD13	15	0.18
(1,173)	2:B:368:LEU:HD11	2:B:369:ASP:H	9	0.18
(1,173)	2:B:368:LEU:HD12	2:B:369:ASP:H	9	0.18
(1,173)	2:B:368:LEU:HD13	2:B:369:ASP:H	9	0.18
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD11	17	0.18
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD12	17	0.18
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD13	17	0.18
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD11	17	0.18
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD12	17	0.18
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD13	17	0.18
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD11	17	0.18
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD12	17	0.18
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD13	17	0.18
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD11	17	0.18
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD12	17	0.18
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD13	17	0.18
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD11	17	0.18
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD12	17	0.18
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD13	17	0.18
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD11	17	0.18
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD12	17	0.18
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD13	17	0.18
(1,871)	1:A:151:PHE:HZ	2:B:402:LYS:HD2	9	0.17
(1,871)	1:A:151:PHE:HZ	2:B:402:LYS:HD3	9	0.17
(1,605)	2:B:355:ILE:HD11	2:B:358:GLU:HB2	12	0.17
(1,605)	2:B:355:ILE:HD12	2:B:358:GLU:HB2	12	0.17
(1,605)	2:B:355:ILE:HD13	2:B:358:GLU:HB2	12	0.17
(1,595)	2:B:403:ILE:HG21	2:B:406:PHE:HB2	16	0.17
(1,595)	2:B:403:ILE:HG22	2:B:406:PHE:HB2	16	0.17
(1,595)	2:B:403:ILE:HG23	2:B:406:PHE:HB2	16	0.17
(1,496)	2:B:406:PHE:HE1	2:B:412:ILE:HD11	1	0.17
(1,496)	2:B:406:PHE:HE1	2:B:412:ILE:HD12	1	0.17
(1,496)	2:B:406:PHE:HE1	2:B:412:ILE:HD13	1	0.17
(1,496)	2:B:406:PHE:HE2	2:B:412:ILE:HD11	1	0.17
(1,496)	2:B:406:PHE:HE2	2:B:412:ILE:HD12	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	2:B:406:PHE:HE2	2:B:412:ILE:HD13	1	0.17
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE1	20	0.17
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE2	20	0.17
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE3	20	0.17
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE1	20	0.17
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE2	20	0.17
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE3	20	0.17
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE1	20	0.17
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE2	20	0.17
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE3	20	0.17
(1,173)	2:B:368:LEU:HD11	2:B:369:ASP:H	7	0.17
(1,173)	2:B:368:LEU:HD12	2:B:369:ASP:H	7	0.17
(1,173)	2:B:368:LEU:HD13	2:B:369:ASP:H	7	0.17
(1,1269)	2:B:411:VAL:HG11	2:B:415:LYS:HD2	12	0.17
(1,1269)	2:B:411:VAL:HG11	2:B:415:LYS:HD3	12	0.17
(1,1269)	2:B:411:VAL:HG12	2:B:415:LYS:HD2	12	0.17
(1,1269)	2:B:411:VAL:HG12	2:B:415:LYS:HD3	12	0.17
(1,1269)	2:B:411:VAL:HG13	2:B:415:LYS:HD2	12	0.17
(1,1269)	2:B:411:VAL:HG13	2:B:415:LYS:HD3	12	0.17
(1,1269)	2:B:411:VAL:HG21	2:B:415:LYS:HD2	12	0.17
(1,1269)	2:B:411:VAL:HG21	2:B:415:LYS:HD3	12	0.17
(1,1269)	2:B:411:VAL:HG22	2:B:415:LYS:HD2	12	0.17
(1,1269)	2:B:411:VAL:HG22	2:B:415:LYS:HD3	12	0.17
(1,1269)	2:B:411:VAL:HG23	2:B:415:LYS:HD2	12	0.17
(1,1269)	2:B:411:VAL:HG23	2:B:415:LYS:HD3	12	0.17
(1,1269)	2:B:411:VAL:HG11	2:B:415:LYS:HD2	15	0.17
(1,1269)	2:B:411:VAL:HG11	2:B:415:LYS:HD3	15	0.17
(1,1269)	2:B:411:VAL:HG12	2:B:415:LYS:HD2	15	0.17
(1,1269)	2:B:411:VAL:HG12	2:B:415:LYS:HD3	15	0.17
(1,1269)	2:B:411:VAL:HG13	2:B:415:LYS:HD2	15	0.17
(1,1269)	2:B:411:VAL:HG13	2:B:415:LYS:HD3	15	0.17
(1,1269)	2:B:411:VAL:HG21	2:B:415:LYS:HD2	15	0.17
(1,1269)	2:B:411:VAL:HG21	2:B:415:LYS:HD3	15	0.17
(1,1269)	2:B:411:VAL:HG22	2:B:415:LYS:HD2	15	0.17
(1,1269)	2:B:411:VAL:HG22	2:B:415:LYS:HD3	15	0.17
(1,1269)	2:B:411:VAL:HG23	2:B:415:LYS:HD2	15	0.17
(1,1269)	2:B:411:VAL:HG23	2:B:415:LYS:HD3	15	0.17
(1,1019)	2:B:362:SER:HA	2:B:364:LYS:HG2	16	0.17
(1,1019)	2:B:362:SER:HA	2:B:364:LYS:HG3	16	0.17
(1,851)	2:B:348:MET:HA	2:B:351:ARG:HD2	20	0.16
(1,851)	2:B:348:MET:HA	2:B:351:ARG:HD3	20	0.16
(1,39)	1:A:148:PHE:H	1:A:149:LEU:HB2	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:A:148:PHE:H	1:A:149:LEU:HB3	19	0.16
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD11	17	0.16
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD12	17	0.16
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD13	17	0.16
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD21	17	0.16
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD22	17	0.16
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD23	17	0.16
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD11	17	0.16
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD12	17	0.16
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD13	17	0.16
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD21	17	0.16
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD22	17	0.16
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD23	17	0.16
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD11	17	0.16
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD12	17	0.16
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD13	17	0.16
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD21	17	0.16
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD22	17	0.16
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD23	17	0.16
(1,1029)	2:B:363:LEU:HD11	2:B:370:VAL:HA	8	0.16
(1,1029)	2:B:363:LEU:HD12	2:B:370:VAL:HA	8	0.16
(1,1029)	2:B:363:LEU:HD13	2:B:370:VAL:HA	8	0.16
(1,1029)	2:B:363:LEU:HD21	2:B:370:VAL:HA	8	0.16
(1,1029)	2:B:363:LEU:HD22	2:B:370:VAL:HA	8	0.16
(1,1029)	2:B:363:LEU:HD23	2:B:370:VAL:HA	8	0.16
(1,692)	2:B:407:LYS:H	2:B:407:LYS:HG2	16	0.15
(1,692)	2:B:407:LYS:H	2:B:407:LYS:HG3	16	0.15
(1,173)	2:B:368:LEU:HD11	2:B:369:ASP:H	11	0.15
(1,173)	2:B:368:LEU:HD12	2:B:369:ASP:H	11	0.15
(1,173)	2:B:368:LEU:HD13	2:B:369:ASP:H	11	0.15
(1,1307)	2:B:423:PHE:H	2:B:424:LYS:HG2	16	0.15
(1,1307)	2:B:423:PHE:H	2:B:424:LYS:HG3	16	0.15
(1,825)	2:B:407:LYS:HA	2:B:413:MET:HG2	5	0.14
(1,77)	1:A:148:PHE:HD1	1:A:149:LEU:H	20	0.14
(1,77)	1:A:148:PHE:HD2	1:A:149:LEU:H	20	0.14
(1,675)	2:B:348:MET:HE1	2:B:385:VAL:HG11	18	0.14
(1,675)	2:B:348:MET:HE1	2:B:385:VAL:HG12	18	0.14
(1,675)	2:B:348:MET:HE1	2:B:385:VAL:HG13	18	0.14
(1,675)	2:B:348:MET:HE2	2:B:385:VAL:HG11	18	0.14
(1,675)	2:B:348:MET:HE2	2:B:385:VAL:HG12	18	0.14
(1,675)	2:B:348:MET:HE2	2:B:385:VAL:HG13	18	0.14
(1,675)	2:B:348:MET:HE3	2:B:385:VAL:HG11	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	2:B:348:MET:HE3	2:B:385:VAL:HG12	18	0.14
(1,675)	2:B:348:MET:HE3	2:B:385:VAL:HG13	18	0.14
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE1	13	0.14
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE2	13	0.14
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE3	13	0.14
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE1	13	0.14
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE2	13	0.14
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE3	13	0.14
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE1	13	0.14
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE2	13	0.14
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE3	13	0.14
(1,413)	2:B:350:SER:H	2:B:352:LEU:HB2	20	0.14
(1,398)	2:B:406:PHE:HD1	2:B:408:VAL:HG21	11	0.14
(1,398)	2:B:406:PHE:HD1	2:B:408:VAL:HG22	11	0.14
(1,398)	2:B:406:PHE:HD1	2:B:408:VAL:HG23	11	0.14
(1,398)	2:B:406:PHE:HD2	2:B:408:VAL:HG21	11	0.14
(1,398)	2:B:406:PHE:HD2	2:B:408:VAL:HG22	11	0.14
(1,398)	2:B:406:PHE:HD2	2:B:408:VAL:HG23	11	0.14
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD11	2	0.14
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD12	2	0.14
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD13	2	0.14
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD11	2	0.14
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD12	2	0.14
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD13	2	0.14
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD11	2	0.14
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD12	2	0.14
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD13	2	0.14
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD11	2	0.14
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD12	2	0.14
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD13	2	0.14
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD11	2	0.14
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD12	2	0.14
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD13	2	0.14
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD11	2	0.14
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD12	2	0.14
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD13	2	0.14
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD11	3	0.14
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD12	3	0.14
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD13	3	0.14
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD11	3	0.14
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD12	3	0.14
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD13	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD11	3	0.14
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD12	3	0.14
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD13	3	0.14
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD11	3	0.14
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD12	3	0.14
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD13	3	0.14
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD11	3	0.14
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD12	3	0.14
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD13	3	0.14
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD11	3	0.14
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD12	3	0.14
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD13	3	0.14
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD11	10	0.14
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD12	10	0.14
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD13	10	0.14
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD21	10	0.14
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD22	10	0.14
(1,1052)	2:B:368:LEU:HA	2:B:368:LEU:HD23	10	0.14
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE1	5	0.13
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE2	5	0.13
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE3	5	0.13
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE1	5	0.13
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE2	5	0.13
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE3	5	0.13
(1,864)	2:B:349:ASP:HA	2:B:352:LEU:HB3	16	0.13
(1,837)	2:B:361:ASN:HA	2:B:364:LYS:HE2	20	0.13
(1,837)	2:B:361:ASN:HA	2:B:364:LYS:HE3	20	0.13
(1,483)	2:B:363:LEU:HD11	2:B:412:ILE:HD11	6	0.13
(1,483)	2:B:363:LEU:HD11	2:B:412:ILE:HD12	6	0.13
(1,483)	2:B:363:LEU:HD11	2:B:412:ILE:HD13	6	0.13
(1,483)	2:B:363:LEU:HD12	2:B:412:ILE:HD11	6	0.13
(1,483)	2:B:363:LEU:HD12	2:B:412:ILE:HD12	6	0.13
(1,483)	2:B:363:LEU:HD12	2:B:412:ILE:HD13	6	0.13
(1,483)	2:B:363:LEU:HD13	2:B:412:ILE:HD11	6	0.13
(1,483)	2:B:363:LEU:HD13	2:B:412:ILE:HD12	6	0.13
(1,483)	2:B:363:LEU:HD13	2:B:412:ILE:HD13	6	0.13
(1,173)	2:B:368:LEU:HD11	2:B:369:ASP:H	19	0.13
(1,173)	2:B:368:LEU:HD12	2:B:369:ASP:H	19	0.13
(1,173)	2:B:368:LEU:HD13	2:B:369:ASP:H	19	0.13
(1,173)	2:B:368:LEU:HD11	2:B:369:ASP:H	20	0.13
(1,173)	2:B:368:LEU:HD12	2:B:369:ASP:H	20	0.13
(1,173)	2:B:368:LEU:HD13	2:B:369:ASP:H	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	2:B:368:LEU:HG	2:B:369:ASP:H	16	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG11	7	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG12	7	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG13	7	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG21	7	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG22	7	0.13
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG23	7	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG11	7	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG12	7	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG13	7	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG21	7	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG22	7	0.13
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG23	7	0.13
(1,1055)	2:B:368:LEU:HD11	2:B:406:PHE:HE1	4	0.13
(1,1055)	2:B:368:LEU:HD11	2:B:406:PHE:HE2	4	0.13
(1,1055)	2:B:368:LEU:HD12	2:B:406:PHE:HE1	4	0.13
(1,1055)	2:B:368:LEU:HD12	2:B:406:PHE:HE2	4	0.13
(1,1055)	2:B:368:LEU:HD13	2:B:406:PHE:HE1	4	0.13
(1,1055)	2:B:368:LEU:HD13	2:B:406:PHE:HE2	4	0.13
(1,1055)	2:B:368:LEU:HD21	2:B:406:PHE:HE1	4	0.13
(1,1055)	2:B:368:LEU:HD21	2:B:406:PHE:HE2	4	0.13
(1,1055)	2:B:368:LEU:HD22	2:B:406:PHE:HE1	4	0.13
(1,1055)	2:B:368:LEU:HD22	2:B:406:PHE:HE2	4	0.13
(1,1055)	2:B:368:LEU:HD23	2:B:406:PHE:HE1	4	0.13
(1,1055)	2:B:368:LEU:HD23	2:B:406:PHE:HE2	4	0.13
(1,686)	2:B:421:ASN:HA	2:B:424:LYS:HD2	15	0.12
(1,625)	2:B:351:ARG:HG2	2:B:383:LEU:HD11	20	0.12
(1,625)	2:B:351:ARG:HG2	2:B:383:LEU:HD12	20	0.12
(1,625)	2:B:351:ARG:HG2	2:B:383:LEU:HD13	20	0.12
(1,608)	2:B:352:LEU:HA	2:B:355:ILE:HD11	15	0.12
(1,608)	2:B:352:LEU:HA	2:B:355:ILE:HD12	15	0.12
(1,608)	2:B:352:LEU:HA	2:B:355:ILE:HD13	15	0.12
(1,452)	2:B:393:HIS:H	2:B:396:MET:HE1	16	0.12
(1,452)	2:B:393:HIS:H	2:B:396:MET:HE2	16	0.12
(1,452)	2:B:393:HIS:H	2:B:396:MET:HE3	16	0.12
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE1	17	0.12
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE2	17	0.12
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE3	17	0.12
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE1	17	0.12
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE2	17	0.12
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE3	17	0.12
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE1	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE2	17	0.12
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE3	17	0.12
(1,39)	1:A:148:PHE:H	1:A:149:LEU:HB2	16	0.12
(1,39)	1:A:148:PHE:H	1:A:149:LEU:HB3	16	0.12
(1,1293)	2:B:419:LEU:HD11	2:B:422:LYS:HE2	9	0.12
(1,1293)	2:B:419:LEU:HD11	2:B:422:LYS:HE3	9	0.12
(1,1293)	2:B:419:LEU:HD12	2:B:422:LYS:HE2	9	0.12
(1,1293)	2:B:419:LEU:HD12	2:B:422:LYS:HE3	9	0.12
(1,1293)	2:B:419:LEU:HD13	2:B:422:LYS:HE2	9	0.12
(1,1293)	2:B:419:LEU:HD13	2:B:422:LYS:HE3	9	0.12
(1,1293)	2:B:419:LEU:HD21	2:B:422:LYS:HE2	9	0.12
(1,1293)	2:B:419:LEU:HD21	2:B:422:LYS:HE3	9	0.12
(1,1293)	2:B:419:LEU:HD22	2:B:422:LYS:HE2	9	0.12
(1,1293)	2:B:419:LEU:HD22	2:B:422:LYS:HE3	9	0.12
(1,1293)	2:B:419:LEU:HD23	2:B:422:LYS:HE2	9	0.12
(1,1293)	2:B:419:LEU:HD23	2:B:422:LYS:HE3	9	0.12
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG11	13	0.12
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG12	13	0.12
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG13	13	0.12
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG21	13	0.12
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG22	13	0.12
(1,1257)	2:B:410:GLN:HG2	2:B:411:VAL:HG23	13	0.12
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG11	13	0.12
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG12	13	0.12
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG13	13	0.12
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG21	13	0.12
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG22	13	0.12
(1,1257)	2:B:410:GLN:HG3	2:B:411:VAL:HG23	13	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD11	1	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD12	1	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD13	1	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD21	1	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD22	1	0.12
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD23	1	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD11	1	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD12	1	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD13	1	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD21	1	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD22	1	0.12
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD23	1	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD11	1	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD12	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD13	1	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD21	1	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD22	1	0.12
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD23	1	0.12
(1,1121)	2:B:377:LEU:HD11	2:B:415:LYS:HE2	13	0.12
(1,1121)	2:B:377:LEU:HD11	2:B:415:LYS:HE3	13	0.12
(1,1121)	2:B:377:LEU:HD12	2:B:415:LYS:HE2	13	0.12
(1,1121)	2:B:377:LEU:HD12	2:B:415:LYS:HE3	13	0.12
(1,1121)	2:B:377:LEU:HD13	2:B:415:LYS:HE2	13	0.12
(1,1121)	2:B:377:LEU:HD13	2:B:415:LYS:HE3	13	0.12
(1,1121)	2:B:377:LEU:HD21	2:B:415:LYS:HE2	13	0.12
(1,1121)	2:B:377:LEU:HD21	2:B:415:LYS:HE3	13	0.12
(1,1121)	2:B:377:LEU:HD22	2:B:415:LYS:HE2	13	0.12
(1,1121)	2:B:377:LEU:HD22	2:B:415:LYS:HE3	13	0.12
(1,1121)	2:B:377:LEU:HD23	2:B:415:LYS:HE2	13	0.12
(1,1121)	2:B:377:LEU:HD23	2:B:415:LYS:HE3	13	0.12
(1,933)	1:A:147:GLN:HB2	1:A:149:LEU:HD11	7	0.11
(1,933)	1:A:147:GLN:HB2	1:A:149:LEU:HD12	7	0.11
(1,933)	1:A:147:GLN:HB2	1:A:149:LEU:HD13	7	0.11
(1,933)	1:A:147:GLN:HB2	1:A:149:LEU:HD21	7	0.11
(1,933)	1:A:147:GLN:HB2	1:A:149:LEU:HD22	7	0.11
(1,933)	1:A:147:GLN:HB2	1:A:149:LEU:HD23	7	0.11
(1,933)	1:A:147:GLN:HB3	1:A:149:LEU:HD11	7	0.11
(1,933)	1:A:147:GLN:HB3	1:A:149:LEU:HD12	7	0.11
(1,933)	1:A:147:GLN:HB3	1:A:149:LEU:HD13	7	0.11
(1,933)	1:A:147:GLN:HB3	1:A:149:LEU:HD21	7	0.11
(1,933)	1:A:147:GLN:HB3	1:A:149:LEU:HD22	7	0.11
(1,933)	1:A:147:GLN:HB3	1:A:149:LEU:HD23	7	0.11
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE1	4	0.11
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE2	4	0.11
(1,892)	2:B:407:LYS:HD2	2:B:413:MET:HE3	4	0.11
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE1	4	0.11
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE2	4	0.11
(1,892)	2:B:407:LYS:HD3	2:B:413:MET:HE3	4	0.11
(1,74)	1:A:148:PHE:HE1	2:B:363:LEU:HG	17	0.11
(1,74)	1:A:148:PHE:HE2	2:B:363:LEU:HG	17	0.11
(1,56)	1:A:151:PHE:HD1	2:B:360:LYS:HA	20	0.11
(1,56)	1:A:151:PHE:HD2	2:B:360:LYS:HA	20	0.11
(1,527)	2:B:370:VAL:H	2:B:370:VAL:HG11	15	0.11
(1,527)	2:B:370:VAL:H	2:B:370:VAL:HG12	15	0.11
(1,527)	2:B:370:VAL:H	2:B:370:VAL:HG13	15	0.11
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE1	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE2	19	0.11
(1,433)	2:B:386:THR:HG21	2:B:426:MET:HE3	19	0.11
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE1	19	0.11
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE2	19	0.11
(1,433)	2:B:386:THR:HG22	2:B:426:MET:HE3	19	0.11
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE1	19	0.11
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE2	19	0.11
(1,433)	2:B:386:THR:HG23	2:B:426:MET:HE3	19	0.11
(1,386)	2:B:420:TYR:HE1	2:B:421:ASN:H	13	0.11
(1,386)	2:B:420:TYR:HE2	2:B:421:ASN:H	13	0.11
(1,319)	2:B:406:PHE:HB2	2:B:407:LYS:H	5	0.11
(1,311)	2:B:405:ARG:H	2:B:406:PHE:HB2	3	0.11
(1,311)	2:B:405:ARG:H	2:B:406:PHE:HB2	15	0.11
(1,173)	2:B:368:LEU:HD11	2:B:369:ASP:H	2	0.11
(1,173)	2:B:368:LEU:HD12	2:B:369:ASP:H	2	0.11
(1,173)	2:B:368:LEU:HD13	2:B:369:ASP:H	2	0.11
(1,173)	2:B:368:LEU:HD11	2:B:369:ASP:H	17	0.11
(1,173)	2:B:368:LEU:HD12	2:B:369:ASP:H	17	0.11
(1,173)	2:B:368:LEU:HD13	2:B:369:ASP:H	17	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD11	2	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD12	2	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD13	2	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD21	2	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD22	2	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD23	2	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD11	2	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD12	2	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD13	2	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD21	2	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD22	2	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD23	2	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD11	2	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD12	2	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD13	2	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD21	2	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD22	2	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD23	2	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD11	5	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD12	5	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD13	5	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD21	5	0.11
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD22	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	2:B:397:ILE:HD11	2:B:400:LEU:HD23	5	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD11	5	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD12	5	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD13	5	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD21	5	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD22	5	0.11
(1,1206)	2:B:397:ILE:HD12	2:B:400:LEU:HD23	5	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD11	5	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD12	5	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD13	5	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD21	5	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD22	5	0.11
(1,1206)	2:B:397:ILE:HD13	2:B:400:LEU:HD23	5	0.11
(1,1196)	2:B:394:THR:HG21	2:B:397:ILE:HG12	20	0.11
(1,1196)	2:B:394:THR:HG21	2:B:397:ILE:HG13	20	0.11
(1,1196)	2:B:394:THR:HG22	2:B:397:ILE:HG12	20	0.11
(1,1196)	2:B:394:THR:HG22	2:B:397:ILE:HG13	20	0.11
(1,1196)	2:B:394:THR:HG23	2:B:397:ILE:HG12	20	0.11
(1,1196)	2:B:394:THR:HG23	2:B:397:ILE:HG13	20	0.11
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD11	14	0.11
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD12	14	0.11
(1,1066)	2:B:370:VAL:HG11	2:B:374:ILE:HD13	14	0.11
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD11	14	0.11
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD12	14	0.11
(1,1066)	2:B:370:VAL:HG12	2:B:374:ILE:HD13	14	0.11
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD11	14	0.11
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD12	14	0.11
(1,1066)	2:B:370:VAL:HG13	2:B:374:ILE:HD13	14	0.11
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD11	14	0.11
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD12	14	0.11
(1,1066)	2:B:370:VAL:HG21	2:B:374:ILE:HD13	14	0.11
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD11	14	0.11
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD12	14	0.11
(1,1066)	2:B:370:VAL:HG22	2:B:374:ILE:HD13	14	0.11
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD11	14	0.11
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD12	14	0.11
(1,1066)	2:B:370:VAL:HG23	2:B:374:ILE:HD13	14	0.11
(1,1002)	2:B:358:GLU:HG2	2:B:376:ALA:HB1	18	0.11
(1,1002)	2:B:358:GLU:HG2	2:B:376:ALA:HB2	18	0.11
(1,1002)	2:B:358:GLU:HG2	2:B:376:ALA:HB3	18	0.11
(1,1002)	2:B:358:GLU:HG3	2:B:376:ALA:HB1	18	0.11
(1,1002)	2:B:358:GLU:HG3	2:B:376:ALA:HB2	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	2:B:358:GLU:HG3	2:B:376:ALA:HB3	18	0.11

10 Dihedral-angle violation analysis

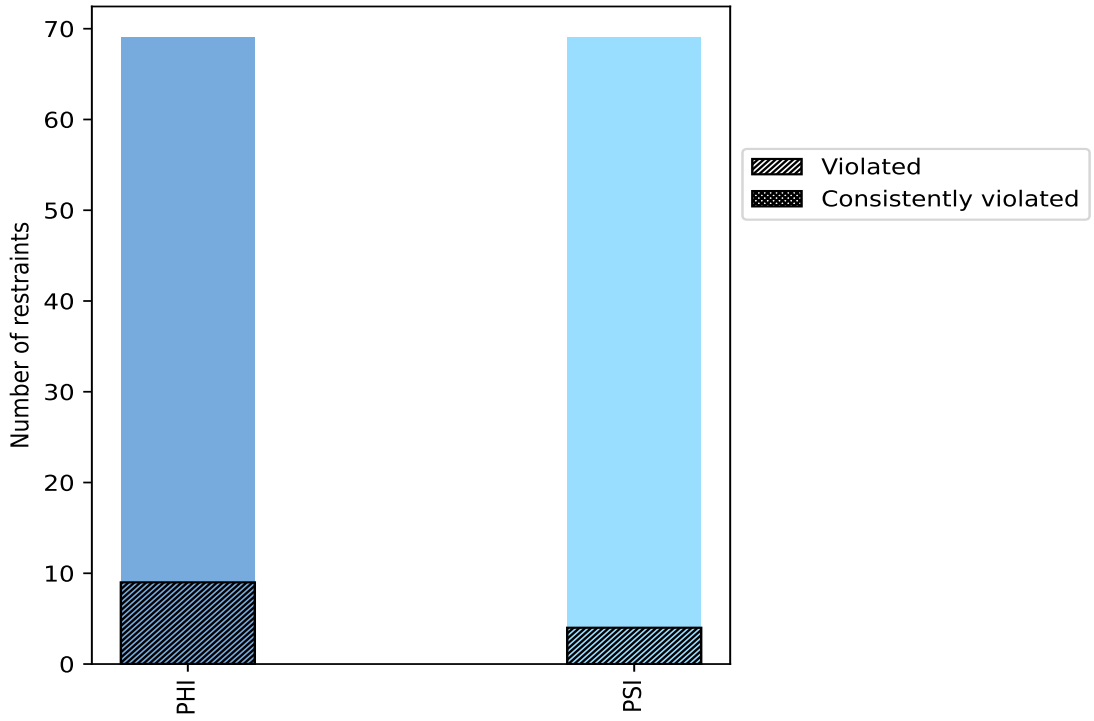
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	69	50.0	9	13.0	6.5	0	0.0	0.0
PSI	69	50.0	4	5.8	2.9	0	0.0	0.0
Total	138	100.0	13	9.4	9.4	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



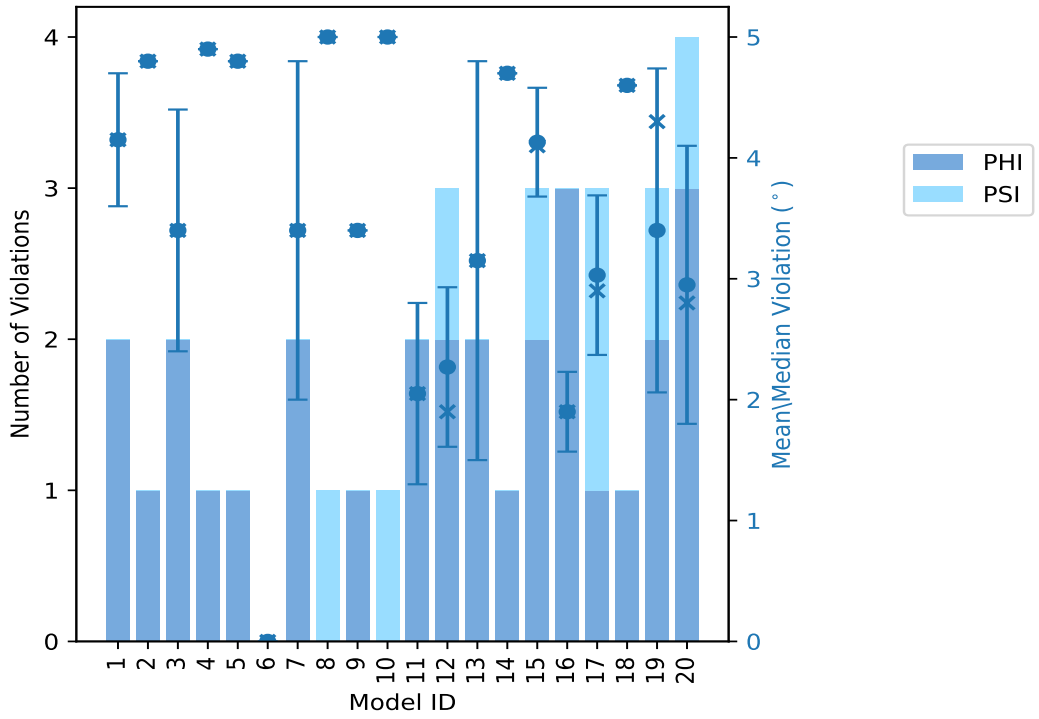
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	2	0	2	4.15	4.7	0.55	4.15
2	1	0	1	4.8	4.8	0.0	4.8
3	2	0	2	3.4	4.4	1.0	3.4
4	1	0	1	4.9	4.9	0.0	4.9
5	1	0	1	4.8	4.8	0.0	4.8
6	0	0	0	0.0	0.0	0.0	0.0
7	2	0	2	3.4	4.8	1.4	3.4
8	0	1	1	5.0	5.0	0.0	5.0
9	1	0	1	3.4	3.4	0.0	3.4
10	0	1	1	5.0	5.0	0.0	5.0
11	2	0	2	2.05	2.8	0.75	2.05
12	2	1	3	2.27	3.2	0.66	1.9
13	2	0	2	3.15	4.8	1.65	3.15
14	1	0	1	4.7	4.7	0.0	4.7
15	2	1	3	4.13	4.7	0.45	4.1
16	3	0	3	1.9	2.3	0.33	1.9
17	1	2	3	3.03	3.9	0.66	2.9
18	1	0	1	4.6	4.6	0.0	4.6
19	2	1	3	3.4	4.4	1.34	4.3
20	3	1	4	2.95	4.5	1.15	2.8

10.2.1 Bar graph : Dihedral violation statistics for each model



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
2	2	4	1	5.0
3	1	4	2	10.0
2	0	2	3	15.0
0	1	1	4	20.0
1	0	1	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

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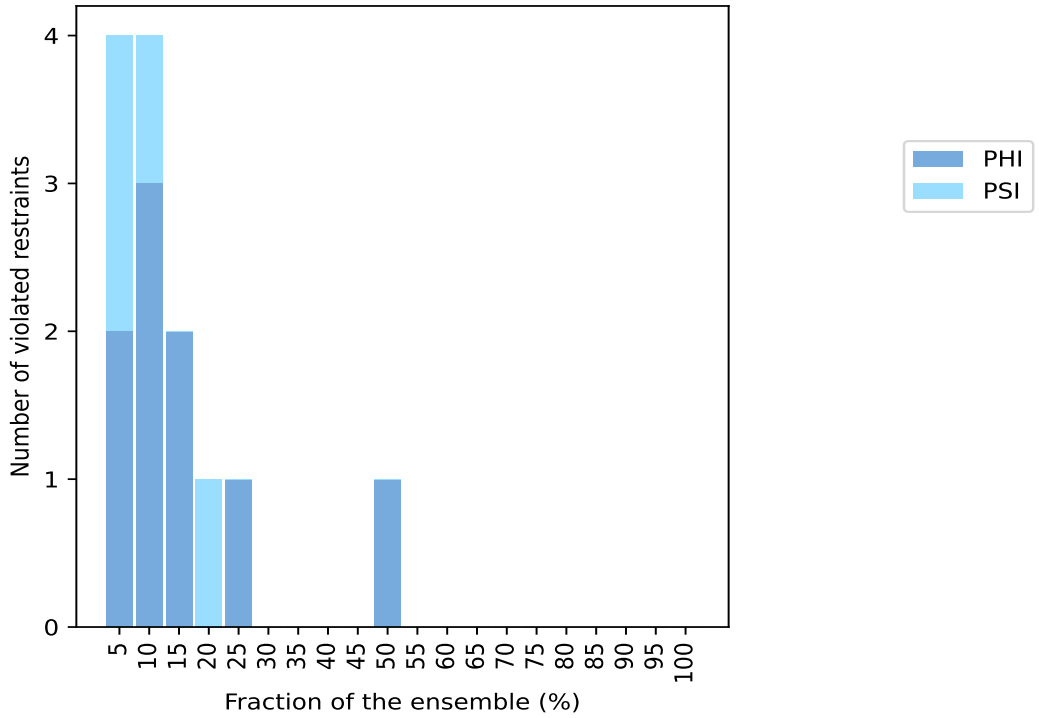
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

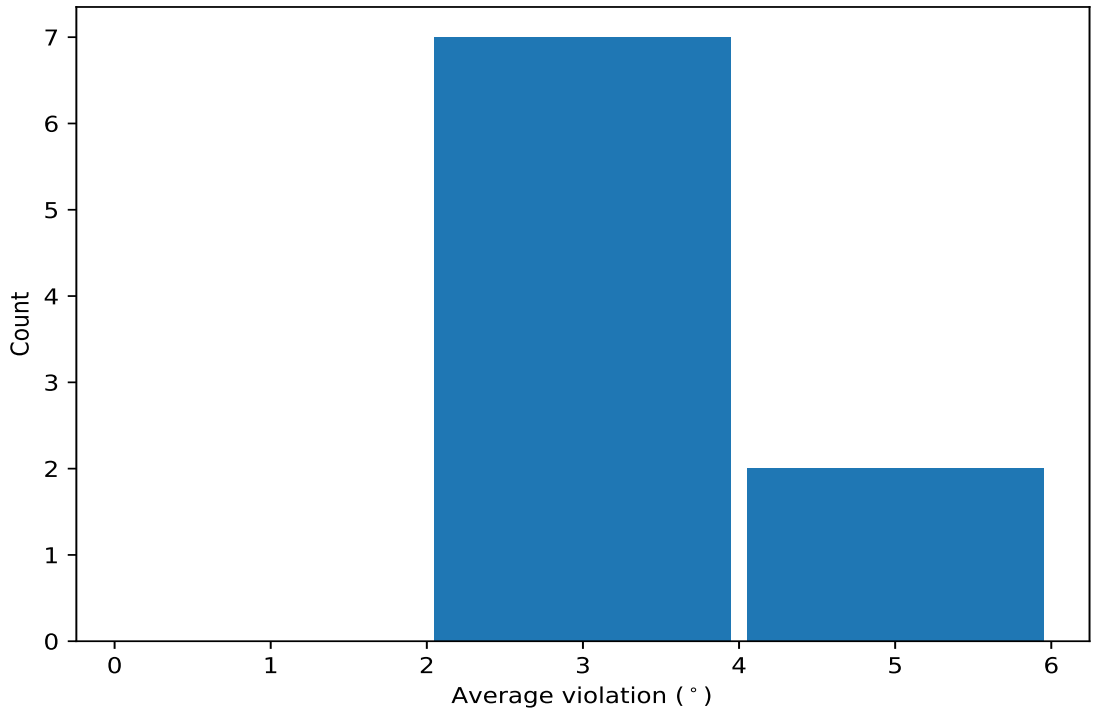


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

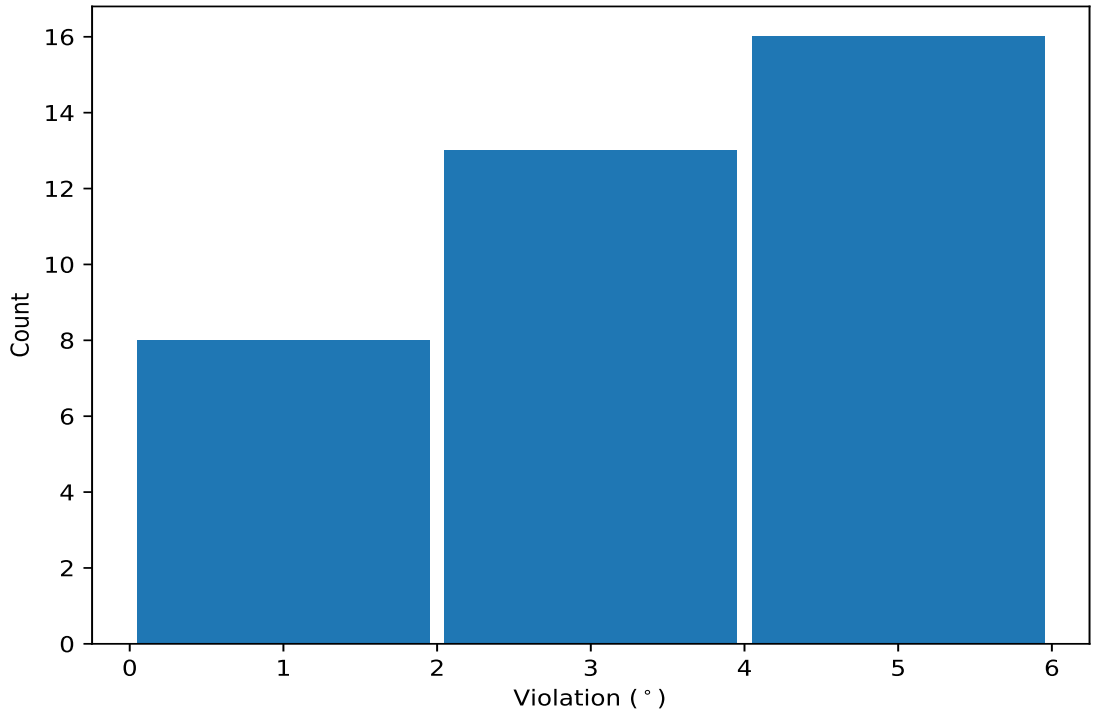
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	10	3.8	1.31	4.5
(1,63)	2:B:381:ALA:C	2:B:382:SER:N	2:B:382:SER:CA	2:B:382:SER:C	5	3.04	0.81	2.9
(1,10)	2:B:352:LEU:N	2:B:352:LEU:CA	2:B:352:LEU:C	2:B:353:GLN:N	4	3.62	0.95	3.6
(1,97)	2:B:401:LYS:C	2:B:402:LYS:N	2:B:402:LYS:CA	2:B:402:LYS:C	3	2.9	1.24	2.4
(1,9)	2:B:351:ARG:C	2:B:352:LEU:N	2:B:352:LEU:CA	2:B:352:LEU:C	3	2.77	1.45	2.0
(1,1)	2:B:347:SER:C	2:B:348:MET:N	2:B:348:MET:CA	2:B:348:MET:C	2	4.05	0.65	4.05
(1,7)	2:B:350:SER:C	2:B:351:ARG:N	2:B:351:ARG:CA	2:B:351:ARG:C	2	4.0	0.4	4.0
(1,99)	2:B:402:LYS:C	2:B:403:ILE:N	2:B:403:ILE:CA	2:B:403:ILE:C	2	3.1	1.6	3.1
(1,54)	2:B:377:LEU:N	2:B:377:LEU:CA	2:B:377:LEU:C	2:B:378:ASP:N	2	2.9	1.0	2.9

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,84)	2:B:395:GLU:N	2:B:395:GLU:CA	2:B:395:GLU:C	2:B:396:MET:N	10	5.0
(1,10)	2:B:352:LEU:N	2:B:352:LEU:CA	2:B:352:LEU:C	2:B:353:GLN:N	8	5.0
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	4	4.9
(1,9)	2:B:351:ARG:C	2:B:352:LEU:N	2:B:352:LEU:CA	2:B:352:LEU:C	7	4.8
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	2	4.8
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	5	4.8
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	13	4.8
(1,99)	2:B:402:LYS:C	2:B:403:ILE:N	2:B:403:ILE:CA	2:B:403:ILE:C	15	4.7
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	14	4.7
(1,1)	2:B:347:SER:C	2:B:348:MET:N	2:B:348:MET:CA	2:B:348:MET:C	1	4.7
(1,97)	2:B:401:LYS:C	2:B:402:LYS:N	2:B:402:LYS:CA	2:B:402:LYS:C	18	4.6
(1,29)	2:B:361:ASN:C	2:B:362:SER:N	2:B:362:SER:CA	2:B:362:SER:C	20	4.5
(1,7)	2:B:350:SER:C	2:B:351:ARG:N	2:B:351:ARG:CA	2:B:351:ARG:C	19	4.4
(1,63)	2:B:381:ALA:C	2:B:382:SER:N	2:B:382:SER:CA	2:B:382:SER:C	3	4.4
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	19	4.3
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	15	4.1
(1,54)	2:B:377:LEU:N	2:B:377:LEU:CA	2:B:377:LEU:C	2:B:378:ASP:N	17	3.9
(1,7)	2:B:350:SER:C	2:B:351:ARG:N	2:B:351:ARG:CA	2:B:351:ARG:C	1	3.6
(1,10)	2:B:352:LEU:N	2:B:352:LEU:CA	2:B:352:LEU:C	2:B:353:GLN:N	15	3.6
(1,10)	2:B:352:LEU:N	2:B:352:LEU:CA	2:B:352:LEU:C	2:B:353:GLN:N	20	3.6
(1,1)	2:B:347:SER:C	2:B:348:MET:N	2:B:348:MET:CA	2:B:348:MET:C	9	3.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,63)	2:B:381:ALA:C	2:B:382:SER:N	2:B:382:SER:CA	2:B:382:SER:C	12	3.2
(1,63)	2:B:381:ALA:C	2:B:382:SER:N	2:B:382:SER:CA	2:B:382:SER:C	17	2.9
(1,63)	2:B:381:ALA:C	2:B:382:SER:N	2:B:382:SER:CA	2:B:382:SER:C	11	2.8
(1,97)	2:B:401:LYS:C	2:B:402:LYS:N	2:B:402:LYS:CA	2:B:402:LYS:C	3	2.4
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	16	2.3
(1,10)	2:B:352:LEU:N	2:B:352:LEU:CA	2:B:352:LEU:C	2:B:353:GLN:N	17	2.3
(1,9)	2:B:351:ARG:C	2:B:352:LEU:N	2:B:352:LEU:CA	2:B:352:LEU:C	20	2.0
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	7	2.0
(1,63)	2:B:381:ALA:C	2:B:382:SER:N	2:B:382:SER:CA	2:B:382:SER:C	16	1.9
(1,54)	2:B:377:LEU:N	2:B:377:LEU:CA	2:B:377:LEU:C	2:B:378:ASP:N	12	1.9
(1,97)	2:B:401:LYS:C	2:B:402:LYS:N	2:B:402:LYS:CA	2:B:402:LYS:C	12	1.7
(1,37)	2:B:368:LEU:C	2:B:369:ASP:N	2:B:369:ASP:CA	2:B:369:ASP:C	20	1.7
(1,99)	2:B:402:LYS:C	2:B:403:ILE:N	2:B:403:ILE:CA	2:B:403:ILE:C	16	1.5
(1,9)	2:B:351:ARG:C	2:B:352:LEU:N	2:B:352:LEU:CA	2:B:352:LEU:C	13	1.5
(1,101)	2:B:404:ARG:N	2:B:404:ARG:CA	2:B:404:ARG:C	2:B:405:ARG:N	19	1.5
(1,75)	2:B:388:GLN:C	2:B:389:GLN:N	2:B:389:GLN:CA	2:B:389:GLN:C	11	1.3